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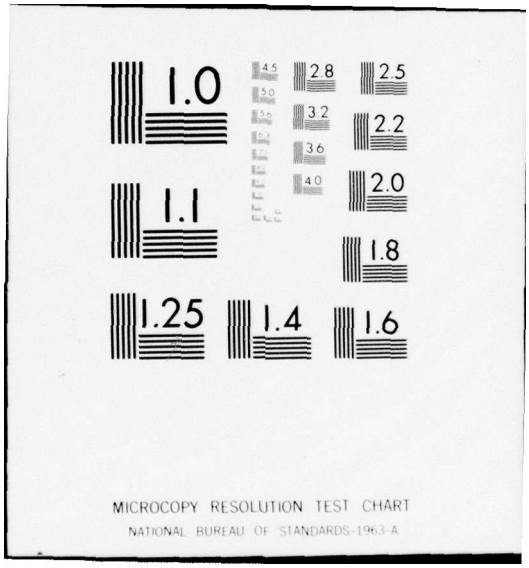
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SAMCEP: A CORRELATED MONTE CARLO NEUTRON AND GAMMA RADIATION TRANSPORT CODE

Prepared by

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February 1977

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)
SAMCEP is a system of U.S.A. - Standard FORTRAN programs for the solution by Monte Carlo of several correlated neutron and secondary gamma transport problems in complex three-dimensional geometries. Up to 10 correlated problems, involving perturbations of composition, neutron cross sections, angular or energy distributions, and/or source spectra, as well as perturbations of gamma production data, can be run simultaneously. Individual problem fluxes (region-, energy-, and time-dependent), as well

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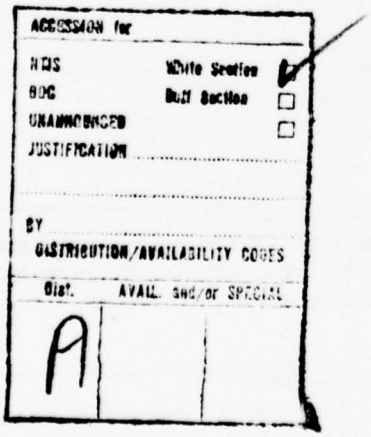
as the flux differences between any or all pairs of problems, are available. In addition, fluxes can be obtained at point detectors, with a built-in biasing procedure to bound the estimates, the so-called bounded flux-at-a-point (BFAP) estimation procedure.

SAMCEP retains essentially all the features of its predecessor code, SAM-CE, including the use of basic element data in the latest ENDF/B format.

This code manual is an extensive revision of the final report for the SAMCEP program originally developed under contract DAAD05-70-C-0295:

> S. Hui, D. Spielberg, H. Steinberg, E. S. Troubetzkoy, M. Kalos, "SAMCEP: An Application of Correlated Monte Carlo to the Simultaneous Solution of Multiple, Perturbed, Time-Dependent Neutron Transport Problems in Complex Three-Dimensional Geometry", BRL CR62, MAGI MR-7020 (January 1972).

Latest revisions reflect the secondary gamma capability with provisions for perturbing the gamma production data, as implemented under the current contract DAAD05-75-C-0735.



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1. INTRODUCTION

SAMCEP is a Monte Carlo neutron and secondary gamma transport code which is designed to calculate differences in fluxes and in flux-derived quantities such as dose, as functions of differences in nuclear data. Source spectral changes can also be considered. SAMCEP is an extension of SAM-CE[1], a general purpose three-dimensional Monte Carlo transport code. SAMCEP, originally developed under contract DAAD-05-70-C-0295*, uses the latest (ENDF/B) cross sections[2,4] to a high degree of precision.

The extension of SAM-CE to SAMCEP involves the addition of the capability of running several similar Monte Carlo problems simultaneously. The mathematical basis of this extension is the simultaneous use, in several correlated problems, of the same Monte Carlo histories, taking account of the effects of the cross section differences via a series of problem-dependent weights associated with each history.

Using SAMCEP, flux differences due to small cross section variations can be calculated much more rapidly and accurately than by conventional methods, i.e., by independent computations. The process of measuring, reducing, evaluating, and communicating nuclear data is slow and expensive. It is essential, therefore, for proper management of such an effort to know whether errors or uncertainties in data result in operationally significant errors or uncertainties in transport computations. SAMCEP is a practical tool that can provide information permitting one to direct cross section research to obtaining more accurate data in those areas where the lack of precision leads to the greatest uncertainty in the transport calculation.

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* The bounded flux-at-a-point capability was developed under DAAD-05-73-C-0072. The secondary gamma capability under DAAD-05-75-C-0735.

In order to describe the capability of SAMCEP, it is necessary first to define a perturbation: a perturbation is a specific change in some portion of the neutron source or changes in the nuclear data for any or all of the elements that make up a medium in a transport problem. SAMCEP can handle, in a single calculation, up to ten correlated problems, each correlated problem including a combination of up to ten perturbations*. The number of allowed perturbations of the neutron data is, therefore, one hundred. (Perturbations of the gamma production data are described in the chapter on PROGRAM SAMGAM).

Perturbations of the neutron data are classified by type as follows:

Type 1	composition (i.e., concentration perturbation); these perturbations carry over to a secondary gamma problem;
Type 2	the complete set of cross section data of an element (i.e., an alternate set of cross section data of a specific element);
Type 3	change of microscopic total cross sections;
Type 4	change of microscopic scattering cross sections;
Type 5	change of microscopic inelastic scattering cross sections;
Type 6	change in angular distribution of elastic scattering;
Type 7	change in secondary energy distribution in continuum inelastic scattering;
Type 8	change in cross sections for inelastic level excitation;
Type 9	change in angular distribution of discrete level inelastic scattering;
Type 10	change in source spectrum

Types 3-9 are defined within specific energy ranges.

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* exclusive of perturbations of the gamma production data for a secondary gamma problem.

SAMCEP consists of five separate programs which may be executed as separate jobs or in sequence as one job. Information is passed from one program to another either by physical tapes or by disk files. (Detailed descriptions of each program and its input data requirements will be given below in separate chapters.) The five programs of SAMCEP are (in the order in which they are executed):

1. Program SAMIN (primary neutron problem) - This program reads the input data describing the neutron perturbations and converts them into the same format as the output of program SAM-X (processor of ENDF/B cross section data[†]).

2. Program SAMSAM (primary neutron problem) - This program reads in the data generated by SAMIN from a tape or a disk file, generates sampling CHI-[*] and ENN-[**] tables when such perturbations exist, (type 2, 6 and 7), and writes such information on a tape or disk file. The other basic function of SAMSAM is to process cross section data into energy band structure by calling subroutine BAND.

[†] The processor SAM-X is a component of the SAM-CE system of programs (Ref. 1).

[*] Table of CHI-boundaries, CHI=(1-cosθ)/2, where θ is scattering angle of equi-probable CHI-bins following elastic scattering.

[**] Table of energy boundaries for equi-probable emerging-energy bins in continuum inelastic scattering.

3. Program SAMCAR (primary neutron and secondary gamma) -

This is the main Monte Carlo program. By calls to a series of independent routines, it performs the following basic functions:

a) process geometry data by calling subroutine GENI,

b) process the unperturbed and perturbed (if any) source spectrum by calling subroutine SOUCAL,

c) perform the transport calculations and score the fluxes by calling subroutine CARLO.

SAMCAR also writes the fluxes by supergroups* of all problems (unperturbed and perturbed) for each aggregate on a tape or a disk file to be edited by the next program SAMOUT.

All neutron perturbation data will be stored in core memory all the time (except for perturbation type 2) and in the same format as the unperturbed data which is the output of SAM-X (processor of ENDF/B data). For perturbation type 2, where an alternate set of cross section data replaces the unperturbed set, the input is required to have the ENDF/B format. SAM-X and BAND will process this as an additional element. (SAMCAR treats the data as an alternate set for the same element.)

For secondary gamma problems, perturbations of the gamma production data (if any) are incorporated into the external source tape generated by program SAMGAM.

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* The term supergroup refers to a subdivision of the output energy range, analogous to a band, which refers to a cross section energy subdivision. Particles are tracked within a superbin, defined as the intersection of the current band and current supergroup. (Refer to Sec. 5.2.6)

4. Program SAMOUT (primary neutron and secondary gamma) - This program reads in the aggregate tape and processes a statistical tape. It then edits the results of all problems, i.e., it displays these results and deviation estimates of all the problems, and also the differences of these results and the deviation estimates of their differences for all specified pairs of problems.

5. Program SAMGAM (secondary gamma problem) - This is the preprocessor for a secondary gamma problem. It presumes the prior execution of the (SAMIN, SAMSAM, SAMCAR, SAMOUT) sequence for the precursor primary neutron problem, which generates a tape of non-elastic (gamma-producing) neutron interactions. Its principal functions, performed by calling several subroutines, are:

   a) alter neutron perturbation tape, retaining only concentration perturbations (if any), by calling PREP8;

   b) prepare organized gamma interaction cross section tape by calling BANDG;

   c) read in user prepared perturbations of the gamma production data, and

   d) generate external source tape, utilizing the interaction tape of the precursor neutron primary and the (possibly perturbed) gamma production data, by calling SAMSOU.

The execution of program SAMGAM is followed by executions of SAMCAR (in the secondary gamma mode) and SAMOUT to complete the secondary gamma sequence.

2. TECHNICAL BACKGROUND

2.1 Simultaneous Tracking

In order to estimate accurately the differences in problem results, each Monte Carlo history is used to estimate all problems simultaneously. As a result there is a high degree of correlation between the answers computed for the individual problems. Hence, the percentage fluctuations in the differences, due to the randomness inherent in the Monte Carlo, are comparable to those in the individual answers. Therefore, the absolute error in the estimated difference is significantly smaller than the error in the difference of the results of separate, uncorrelated calculations.

The implementation of this procedure, the use of the same history for several problems, sometimes called correlated sampling, is based on the fact that it is always possible to carry out a Monte Carlo calculation using probability distributions other than those that describe the natural stochastic processes of radiation. In doing so, a cumulative product of ratios of natural to altered distributions is calculated as a weight with which an answer is counted. Thus, it is possible to use as 'natural' and 'altered' distributions those derived from alternative data. Several answers may be obtained; one for the distribution actually sampled (with weight equal to one) and others from the ratios of distributions. This can be generalized by sampling from probability density functions not corresponding to any physical problem. The sampling density can be defined as the one which attempts to minimize the statistical uncertainties in the difference of the results of the correlated problems.

In SAMCEP, the sampling transport distribution is defined as the least upper bound of the individual transport distributions. All other sampling distributions (source sampling, and sampling of interaction events) are proper

probability distribution functions. They are, therefore, defined as the renormalized least upper bound (l.u.b.) of the individual distributions*. The various sampling distributions are described in more detail below.

Transport Sampling Distribution

In any region, the natural transport kernel for the ith problem is of the form $F_i \mu^i \exp(-\mu^i s)ds$, where μ^i is the total cross section at the current energy E, for concentrations and cross sections appropriate for the ith problem. The F_i's reflect the previous weight adjustments and transport through previous regions.

The ordinary sampling distribution for all problems i, i=1,n, is the least upper bound or envelope of the individual distributions $F_i \mu^i \exp(-\mu^i s)ds$, which is piece-wise exponential and can, therefore, be selected by the standard methods. For BFAP estimation, this procedure is modified (see Appendix E).

Source Sampling Distribution (neutron transport)**

Each problem i, i=1,n, can have a perturbed source energy distribution $S_i(E)$. The sampling distribution is constructed by first constructing S(E) which is the envelope of all $S_i(E)$, biasing it by constructing $S(E)/W_E(E)$ where $W_E(E)$ are the energy-dependent weights in the source region, and finally renormalizing, obtaining the sampling distribution

$$\tilde{S}(E) = \frac{S(E)/W_E(E)}{\int_0^\infty (S(E')/W_E(E'))dE'} .$$

---

* The use of the least upper bound of the distributions, called the envelope, is motivated by the following considerations: it minimizes the maximum relative weight factor in sampling, and so tends to prevent large variances; and it can be constructed automatically in the course of the calculation, so that a detailed examination of the perturbed data is not necessary.

**An external source tape is generated by SAMGAM for secondary gamma transport.

Interaction Sampling Distributions

Selection of Element: Given an interaction in a region, the first sampling implemented is that of the particular element with which the collision occurred.

Let

μ^i = macroscopic total cross section,

σ_j^i = microscopic total cross section for element j,

C_j^i = element concentration of j^{th} element,

NE = total number of elements

$$\mu^i = \sum_{j=1}^{NE} C_j^i \sigma_j^i, \quad \text{for all i (i=1, total number of problems)}$$

Let p_j^i be the probability of picking element j for the i^{th} problem:

$$p_j^i = \frac{C_j^i \sigma_j^i}{\mu^i} .$$

Then the sampling probability p_j^s for picking element j for collision is the renormalized l.u.b. of the p_j^i

$$p_j^s = \text{MAX}_i \left\lceil \frac{F_i C_j^i \sigma_j^i}{\mu^i} \right\rceil \Big/ \text{NORM for all j,}$$

where $\text{NORM} = \sum_j \text{MAX}_i \left\lceil \frac{F_i C_j^i \sigma_j^i}{\mu^i} \right\rceil$

Selection of Interaction Type: Given an interaction with a particular element, the next selection is the type of interaction to occur. If the microscopic elemental total, scattering and inelastic cross section data are given by σ_t^i, σ_s^i and σ_{in}^i, then

$$\frac{\sigma_a^i}{\sigma_t^i}, \quad \frac{\sigma_e^i}{\sigma_t^i}, \text{ and } \frac{\sigma_{in}^i}{\sigma_t^i}, \text{ where } \sigma_a^i = \sigma_t^i - \sigma_s^i$$

are the probabilities of having absorption, elastic scattering, and inelastic scattering, respectively, for the i^{th} problem. We denote the individual distribution (the i^{th} distribution) by

$$p_r^i = \frac{\sigma_r^i}{\sigma_t^i}, \text{ where r may denote absorption, elastic or inelastic scattering reactions.}$$

Then, again by choosing the envelope of this discrete function, we have for the sampling probability distribution for picking reaction r

$$p_r^s = \frac{\text{MAX}_i [F_i p_r^i]}{\sum_r \text{MAX}_i [F_i p_r^i]}$$

The perturbation weight F_i for the i^{th} problem is then multiplied by p_r^i / p_r^s.

Since we allow perturbation of the σ_{in} cross section and also the cross section for level excitation (type 2, 5 and 8), we have to compute the sampling distribution for picking a level or continuum. This sampling distribution is again the envelope of all the individual distributions. When a certain level or continuum is chosen, the weight is adjusted in the same manner as described above.

Given an elastic scattering, the sampling distribution for the angle of scattering is again constructed as the envelope of the angular distributions corresponding to the different perturbations, and is renormalized. The same applies to the energy distribution of inelastic scattering leading to continuous spectra.

2.2 On Energy Binning of Perturbations

In the course of the main Monte Carlo, at every stage at which a decision is to be made (e.g., distance to a collision element with which a collision occurs, reaction type, angle of scattering, or emerging energy), it is necessary to know which perturbations are in effect for the current neutron energy. For this purpose, the entire energy range of the problem is broken up into energy bins whose boundaries are the set of the upper (EH^i) and lower (EL^i) limits of all the perturbations i (cf. Section 3.2). These (EH^i, EL^i), i=1,n, together with the overall energy limits of the problem EHIGH and ELOW are then sorted in decreasing magnitude and entered into a table (the PETAB-array). Another table (IPBIN-array) is constructed, indicating the numbers of perturbations in the various bins of PETAB-array and also the ID's of these perturbations (the ID's are called IP; cf. Section 3.2). Both PETAB- and IPBIN-arrays are constructed in subroutine PPROCS, which is called by subroutine INPUTP of program SAMIN.

During later Monte Carlo calculations, when a particle enters into collision at energy E, the energy table (PETAB) is consulted to locate the energy bin containing E. Knowing this bin-number, one can obtain all the information on the perturbations affecting energy E from the data in the IPBIN-array.

3. PROGRAM SAMIN: NEUTRON PERTURBATION INPUT PROCESSOR

3.1 General Discussion

SAMIN is a driver program which calls subroutine INPUTP to read in and process the neutron perturbation input data and which writes the following perturbation information on a tape or disk file:

MISTER-SISTER array	processed perturbation input data (refer to storage map of MISTER-array in Appendix C).
NTYP-array	cumulative array of perturbations by type, i.e., NTYP(1)=number of perturbations type 1, NTYP(2)= NTYP(1)+number of perturbations of type 2, etc., finally NTYP(N)=sum of all perturbations of types 1, 2, ..., and N.
LOCLIP	location where perturbation data for a specific element of a specific type begin in MISTER-array. (Refer to storage map of MISTER-array in Appendix C.)
NPROB	total number of problems; i.e., unperturbed plus perturbed problems.
LLNEXT	location of first available storage +1 after elemental perturbation data in MISTER-array. Sampling CHI- and ENN-tables start at location (LLNEXT-1) if such perturbations exist.
MMAX	dimension of MISTER-array.
ELOW	low energy cut-off limit of problems run.
EHIGH	high energy limit of problems run.

PETAB-array	perturbation energy table where PETAB(1)=EHIGH, PETAB(last)=ELOW, intermediate entries including all the perturbation energy limits. (All EH's and EL's, cf. Section 3.2.)
IPBIN-array	perturbation binning table (refer to storage map description of IPBIN-array in Appendix D).
LP	total number of energy bins in PETAB-array.

3.2 Processor INPUTP and Description of Input Data for Program SAMIN

A Description of INPUTP, the Routine for Reading and Processing Perturbation Data and Perturbation-Problem Correspondences

As mentioned previously, 10 types of perturbations are permitted. All of the numerical data for the perturbations are read in by subroutine INPUTP, with the exception of those for perturbations of type 2 (whole element). For this type, only the element (nuclide) identification integers for the basic and perturbing data are specified, and it is assumed that both of these identification integers have been included in the element input to the previously run cross-section-processing program SAM-X.

For many of the input items listed below, e.g., those numbered 1; 4.1b; 4.3-4.5a,b; 4.6a,b; etc., certain input options have been implemented to facilitate the entry of single floating numbers or arrays of floating numbers without repeating the right-justified E+nn punch on the input cards.

Specifically, the first of these options permits the cards calling for the EELOW and EEHIGH of the problem (card 1) and all the perturbation cards calling for an EL and EH (e.g., card 4.3a) to have the (e.g.) E+06 punch omitted, and replaced by *6 in columns 79 and 80 of the pertinent cards. The code then enters EL and EH in memory as the actual constants of the designated data fields,

multiplied by 10^6. In general, for such cards (and others indicated below) the pertinent input quantities are scaled (prior to storage) by 10^{+N} if *N appears in columns 79 and 80, and by 10^{-N} if /N appears in these columns. This scaling is done by subroutine SCALE.

Cards for which this option is provided are indicated in the following data and format description by the entry *N at the right-hand side of the format statement, the * is to be understood as representing * or /, while N an integer or blank; (a non-integer alphanumeric in column 80 will cause a system error since the code scans this column in I1 format). If column 80 has a non-zero numerical entry, the code will do nothing to the quantity in the scaled field unless column 79 contains an * or a /. In the input-data format listings below, the quantities affected by the optional scaling are underlined.

Two other types of optional scaling of input data are provided.

The first of these applies to single arrays of floating numbers such as energies (as in items 4.6b, 4.7c). For most of these data, called for in 7E11.4 format, *N or /M in columns 79 and 80 of the first card of the array will cause all the input numbers to be multiplied (prior to printing and storing) by 10+N or 10-M respectively; an optional P (or any other non-blank character) in column 78 will cause the data in the array to be printed out in a higher-precision format (6E16.6) instead of the normal or default format (10E12.4). This scaling and printing is done in subroutine READ75.

Arrays for which this option is provided are indicated below by the entry P*N at the right-hand side of the page; P stands for any non-blank character, * stands for * or /, and N is the integer for exponent scaling.

Finally, there are several types of data which are read in as coordinated tables (6E11.4, x and y alternating; as in energy, cross section, items 4.3-4.5b, 4.7g; or energy, probability, as in item 4.7i). For most of the input

data of this type, columns 77-80 of the first card in the pertinent read operation may have entered a notation such as *L*N, where each * may independently be * or /, and L and N are integers. Entries in columns 77, 78 scale the x (first, or independent-variable field) and those in columns 79, 80 affect the y (second, or dependent-variable field). Hence E, cards punched as follows:

	Col. 11	Col. 22	Col. 33	Col. 44	Col. 55	Col. 66	77	78	79	80
Card 1	1.0	7.1	1.5	6.1	2.	5.1 ...	*	6	/	3
Card 2	2.5	4.1	3.0	3.1			(blank)			

could cause energies 1.0E+6ev, ..., 3.0E+6ev to be correlated with cross sections of .0071, .0061, ..., .0031 barns, respectively, in portions of the INPUTP code where such scaling is provided.

Either or both of columns 78, 80 may be blank, but neither should contain a non-numeric punch. *Scaling action is taken on a field only if the operator (in* col. 77 for x or 79 for y) is * or /. This scaling is done in subroutine RCTAB. Quantities which may be scaled by using this option are underlined in the format lists below.

INPUT to INPUTP

The following describes the input. The information is summarized in Section 3.3.

Item 1 - EELOW, EEHIGH, ISSW (1, 2, ..., 12); FORMAT (2E11.4,8X,12I1),*N

The first two quantities are the low-energy cut-off and the high-energy limit, both in ev, for tracking in the main Monte Carlo calculation*.

ISSW (1,2,...,12) are "sense switch" digits used for selective debugging and additional information via printouts. Non-zero entries elicit the printouts. At present only indices 1,2,6, and 11 have any effect. These are:

*See Appendix H

ISSW(1): Prints out computed Legendre moments of tabulated angular distributions.

ISSW(2): Prints out entire perturbation-array MASTER* at end of calculation, in several formats.

ISSW(6): Prints out details of ANTERP routine operation, locating abscissa corresponding to specified ordinate (area) in elastic angular distribution.

ISSW(11): Prints out partial MASTER* array, showing unedited problem-to-perturbation-correspondence data. These data are also edited and printed independently of ISSW(11).

Item 2 - NTYP (1,2,...,10); FORMAT (10I5).

Ten integers, indicating the numbers of perturbations present of types 1,2,...,10, respectively.** Any or all of these may be zero. If all are zero, this card is the last one that is required. Otherwise:

Item 3 - For each perturbation KK, where KK=1,2,..., $\sum_{J=1}^{10}$ NTYP(J), a card with

KK, NPROB, (JPROB(L),L=1,NPROB); FORMAT (12I5).

Here KK=perturbation number; NPROB is the number of output problems to be affected by the perturbation ($0 \leq NPROB \leq 10$); and JPROB(L) are the particular problem numbers (all distinct, and each $JPROB \leq 10$). KK must be present; if NPROB=0, subsequent input for that perturbation is limited to a single card.

---

* NOTE: Not to be confused with MASTER array in Program SAMCAR.

** The array is internally transformed to a cumulative one, to conform to the definition of Section 3.1.

These data are followed by cards describing the individual perturbations, as follows.

All data for perturbations of type 1 (if any) must be given first, and numbered (KK) in order from 1 to NTYP(1); those for type 2 (if any) must follow, and be numbered consecutively from NTYP(1)+1 to (NTYP(1) + NTYP(2)); etc. Header cards must be present for each perturbation, with identifiers KK=1,2,...,

$$\sum_{J=1}^{10} \text{NTYP}(J),$$ including those for which NPROB=0 (item 3, above).

For each KK with NPROB=0, no further data are required. Otherwise, the required inputs are as follows: (Items 4.1 - 4.10).

Item 4.1 - Type 1, Composition (Present if NTYP(1)>0).

Here a specific composition (set of concentrations), one of those processed by BAND, is perturbed. Required input:

a) KK, ICOMP, NLM; FORMAT (X,I4,2I5),

KK=perturbation index; (an asterisk or other mark may be punched in column 1 to increase legibility of the data deck);

ICOMP = composition number, as specified for BAND;

NLM = number of elements in composition, as specified for BAND; followed by

b) CONC(1,2,...,NLM); FORMAT (7E11.4), P*N.

These are the NLM concentrations of the elements comprising the composition, in atoms/(barn-cm), given in the same order as provided in the BAND input.

NOTE: In all the following sections (4.2-4.10), it is to be understood that for any perturbation KK for which NPROB=0, no data past the first card are to be supplied.

Item 4.2 - Type 2, Whole Element (Present if NTYP(2)>0)

Here, a specified base-case element is understood to have all its cross section data perturbed in the entire energy range. The perturbed data are those of another specified element present* on the existing element data tape (EDT).

Input:

a) KK, ID1, ID2; FORMAT (X,I4,2I10).

KK = perturbation index;

ID1, ID2 are base-case and perturbation element integer identifiers, e.g., 92235 and 92000. Conventionally an identifier is of the form IZAAA, where IZ is an atomic number and AAA an atomic weight. AAA=000 is frequently used to indicate a natural element (mixture of isotopes).

Items 4.3 - 4.5 - Types 3,4,5: Perturbation, within a specified energy range, of total (σ_t), scattering (σ_s), or inelastic (σ_{in}) microscopic cross sections, respectively, of a specified element.

Here, it is implied that specifying a perturbation of σ_t alone implies a change in the absorption cross section; explicitly changing σ_s alone means changing the elastic and absorption cross sections; and explicitly changing σ_{in} alone means changing the inelastic continuum and the elastic scattering cross sections. These relationships can be understood from Figure 1, below, which indicates the components of the total microscopic cross section; the components in boxes are those which are specified in the basic or perturbation data.

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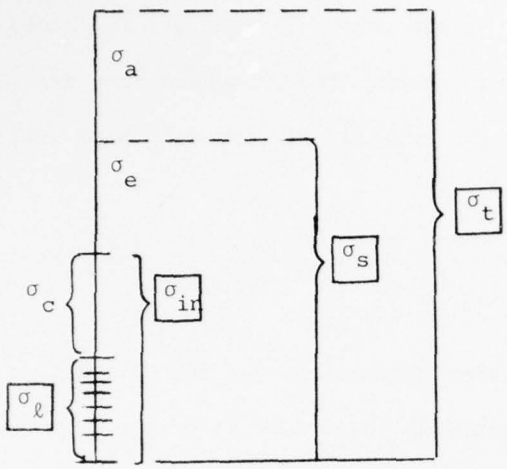
* As the BAND tape is prepared independently of the present input processing, it is required that the BAND input includes the perturbing element. This can be achieved by declaring all perturbing elements to be constituents of a dummy composition (i.e., one which is not referenced by any physical region).



(The level-excitation cross-section σ_ℓ is actually supplied as cross-sections for the excitation of the individual levels.)

Figure 1 - Components of Microscopic Cross-Section

By a suitable superposition of perturbations of types 3,4, and 5 it is possible to specify any desired perturbation. Thus, for example, if it were desired to increase σ_e while leaving σ_a unchanged, this would require simultaneously specifying the required changes (as functions of neutron energy) in σ_s (type 4) and σ_t (type 3).

Required input (types 3, 4 and 5):

For each perturbation present of these types:

a) KK, NEP, JZ, EL, EH, FMULT; FORMAT (X,I4,I5,I10,3E15.5),*N

KK = perturbation index;

NEP = number of energy points at which the cross section is specified (at least 2 for tabulated data; for NEP<2, FMULT is used as the multiplier to be applied to the unperturbed cross sections in the energy range from EL to EH to obtain the perturbed values);

JZ = element identifer as given by SAM-X processor;

EL, EH = low and high energy limits (ev) over which the perturbation is to apply;

FMULT = multiplier for cross sections (used if NEP<2);

next, if NEP≥2 (omit (b) if NEP<2).

b) Supply NEP pairs of (energy (ev), cross-section (barns)):

E(L), σ(L), for L=1,2,...,NEP; FORMAT (6E11.4),*L,*N

The energies and corresponding cross sections are given alternately, 3 pairs to a card, energies in increasing order. As in all the perturbations involving a specified energy range, any supplied table of energies must span the perturbation's EL and EH; i.e., E(1) ≤EL and E(NEP) ≥EH, otherwise the problem stops. The spacing of the energy points should be such that linear interpolation of σ in E is permissible.

Item 4.6 - Type 6, Angular Distribution of Elastic Scattering

Required Input:

a) KK,NE,ID,EL,EH; FORMAT (X,I4,I5,I10,2E15.5),*N.

KK = perturbation index;

NE = number of energy points at which perturbed distributions are supplied;

ID = element identifier;

EL, EH = low and high energy limits (ev) of the perturbation

b) E(L), L=1, NE (energies (ev) in increasing order, for which distributions are given); FORMAT (7E11.4), P*N, (E(1)≤EL, E(NE)≥EH). The spacing of the energies should be such that linear interpolation in energy of the implied distributions is permissible. Next (c-e), CHI-table criteria; one package, applicable for all of the NE energies:

c) LADHOC, N; FORMAT (2I5)

LADHOC, Maximum allowable number of CHI's (equi-probable values of $\chi = \frac{1-\mu}{2}cm$, exclusive of the implied χ=0 and 1), and N, number of Legendre moments of the computed χ-table to be compared with those of the supplied distribution.

LADHOC$\leq$40, N$\leq$50.

If LADHOC = 0: default values will be set internally for LADHOC (=30), N(=3), $\varepsilon_{i=1,2,3}$ (=.02, .02, .02) and α(=.5); where the ε_i and α are defined below.

Skip inputs (d,e), and go to f.

If LADHOC$\geq$1: Let N be the value supplied on card c; then if N=0, skip to (e)(default values of N and ε will be used).

If N>0, supply (d).

d) ε(I), I=1,N FORMAT (10F8.3) (no scaling allowed)

Blank entries for ε, or values <.001, are each replaced internally by .001. The ε are absolute deviations to be allowed in the computed Legendre moments of the χ-table.

$\text{Moment}_j = \int_{-1}^{+1} f(\mu)P_j(\mu)d\mu$, where $f(\mu)=\frac{dp}{d\mu}$ of the supplied (and code-normalized) angular distribution, and $P_j(\mu)$ is the jth Legendre polynomial. The implied moments refer to those beyond the zero-th, which is unity.

e) α FORMAT (E12.4)

α is the fractional deviation to be allowed in the $dp/d\mu$ implied by the generated χ-table, as compared with the maximum value of the supplied distribution, within any one χ-bin. (Actually, the value of the distribution within the χ-table must deviate from the bin-maximum supplied value, and from the average value of the distribution (=.5), by more than α in order for a particular χ-table to be rejected. The ε-tests are the final criteria to be applied.) The code tries χ-tables with more and more CHI's (up to LADHOC) to attempt to satisfy all criteria.

f) LTT; FORMAT (I2)

Type of data supplied, LTT=1 (Legendre coefficient expansion) or LTT=2 (tabulated μ,$dp/d\mu$).

The choice of LTT fixes the type of distribution input for all the input energies.

Next; If LTT=2, skip to Item 4.6.2.

Item 4.6.1 - applies <u>if LTT=1</u>, supply items (g), (h) for each of the NE energies, then skip to Item 4.7.

(g) NL, Number of coefficients (past the zero-th) to be used in the Legendre expansion of the <u>normalized</u> <u>center-of-mass</u> angular distribution $f(\mu)$.

($NL \leq 50$) FORMAT (I5)

(h) $c(L)$, $L=1, NL$; FORMAT (7E11.4) (no scaling allowed)

values of expansion coefficients,

$$c_\ell = \int_{-1}^{+1} f(\mu) P_\ell(\mu) d\mu$$ of the normalized $f(\mu)$, where

$$f(\mu) = \sum_{k=0}^{NL} \frac{2k+1}{2} c_k P_k(\mu); \quad c_o = 1.0$$

$$P_o(\mu) = 1; P_1(\mu) = \mu; \quad P_2(\mu) = \frac{3\mu^2}{2} - \frac{1}{2};$$

$$mP_m(\mu) = (2m-1)\mu P_{m-1}(\mu) - (m-1)P_{m-2}(\mu).$$

Item 4.6.2 - applies if LTT=2. Supply items (i), (j) for each of the NE energies, then enter Item 4.7.

(i) MNP, number of $(\mu, dp/d\mu)$ pairs over range $-1 \leq \mu \leq +1$ supplied to describe center-of-mass angular distribution for particular energy. $(2 \leq MNP \leq 100)$; FORMAT (I5)

j) $(\mu, dp/d\mu)$, (MNP pairs); FORMAT (6E11.4) (no scaling allowed) center-of-mass cosine of scattering angle and probability per unit cosine (differential cross section or probability, not necessarily normalized); μ and $dp/d\mu$, alternately, 3 pairs to a card. The first $dp/d\mu$ should correspond to $\mu=-1.$, the last to $\mu=+1.$; (the code sets $\mu(1)=-1.$ and $\mu(MNP)=+1.$). The spacing should be such that linear interpolation of $dp/d\mu$ in μ is permissible. (Repeat (i) and (j) for each subsequent energy.)

End of Type 6 input.

Item 4.7 - Type 7, Secondary-Energy Distribution of Inelastic Continuum Scattering

Input:

a) KK,NES,ID,EL,EH; FORMAT (X,I4,I5,I10,2E15.5),*N.

KK = perturbation index;

NES = number of energy points at which perturbed distributions are supplied;

ID = element identifier;

EL,EH = low and high energy limits (ev) of the perturbation.

b) NENN(L), L=1 NES; FORMAT (16I5)

These integers are the numbers of ENN (secondary-energy boundaries, defining equally-probably emergent-energy bins) to be generated for each of the NES incoming energies. The values of NENN should be ≥ 2, and non-decreasing (the code corrects the list if necessary to make NENN(1)$\geq$2 and d(NENN)/dL$\geq$0).

c) E(L), L=1, NES; FORMAT (7E11.4),P*N.

NES values of incoming energy, low to high. The list should at least span (EL,EH).

d) NREAC, Number of reactions contributing to the inelastic continuum. FORMAT (I5).

Supply Package (e)-(n) (with appropriate internal choices) for each of the NREAC reactions.

e) KREAC, MT, NK; FORMAT (X,I4,2I5).

Here KREAC is the (required) reaction number (1,2,...,NREAC); MT is the ENDF/B identifier for the reaction type; the allowed values of MT and their meanings are:

MT	Meaning
4	inelastic (n,n')
16	(n,2n)
17	(n,3n)
22	(n,n'α)
23	(n,n'3α)
24	(n,2nα)
25	(n,3nα)
28	(n,n'p)

(use of any other MT will stop the problem); NK is the number of supplied energy distributions, contributing to the total energy distribution for reaction KREAC.

f) NEPS, number of energy points at which the cross section σ_k for reaction KREAC will be supplied.

(NEPS≥2); FORMAT I5)

g) (ES(L), σ_k(L), L=1, NEPS); FORMAT (6E11.4),*L*N

NEPS pairs of (energy, cross section for this reaction); three pairs to a card.

(The energies should be increasing, and spaced so that linear interpolation for σ_k is permissible; the span of energies for σ_k need not encompass EL, EH; for an energy E(L) which lies outside the range of energies for which σ_k is defined, the value of σ_k is taken to be zero.)

Within this reaction-package, supply (h-n) for each of the NK distributions:

h) NEPP, Number of energies at which the probability for this distribution (fraction, p, of σ_k to be associated with this distribution) will be specified (NEPP≥2); FORMAT (I5).

i) (EP(L), P(L), L=1, NEPP); FORMAT (6E11.4),*L*N

Alternate energy, probability for this distribution; 3 pairs to a card, energies increasing. Outside the tabulated range of EP, P is assumed to be zero.

Note: For any one reaction at a specified energy E, the sum of the p's for the various distributions, as obtained by interpolations in E, should equal 1:

$$\sum_{i=1}^{NK} p_i(E) = 1.$$

The code does not check this, so the problem originator should. (Allowing $\sum_i p_i$ to be different from 1 means that the generated energy spectrum is not weighted correctly by σ_k, but effectively by $\sigma_k \cdot \sum p_i$).

The satisfying of this condition ($\sum_i p_i(E)=1$) is facilitated if the same energy mesh is given for all of the tabulated p(E). Then if the condition is satisfied by the p's at each energy mesh point, it will be satisfied by the linearly-interpolated p's at all intermediate energies.

j) LF,U†;FORMAT (I5,E15.4),*N

LF is the energy distribution type; LF=5 or 9; U($\geq$0) is pertinent if LF=9; it is used to truncate an otherwise Maxwellian energy distribution at a maximum E' of E-U. The meanings of the LF's are as follows:

LF=5: Spectrum is supplied as a single table of X,g(X), where X=E'/θ, θ is θ(E), a nuclear temperature, specified as a tabulated function of E, and $g(X)=dn/dX \sim \frac{dn}{dE}$, the probability density of the secondary-energy spectrum;

LF=9: Spectrum is Maxwellian,

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†See M. K. Drake (ed.), "Data Formats and Procedures for the ENDF Neutron Cross Section Library", BNL 50274, ENDF 102, Vol. 1 (1970).

$\frac{dn}{dX} = Xe^{-X}$, up to $X = \frac{E-U}{\theta}$; $\frac{dn}{dX} = 0$ for $X > \frac{E-U}{\theta}$,

where U is constant for all incoming energies E, and θ is a tabulated function of E.

The code generates the required normalization for both cases LF=5 and LF=9, so that

$$\int_0^{E_{max}} \frac{dn}{dE'}\, dE' = 1.$$

If a particular table of g(X) (LF=5) does not extend to high enough X for a particular E to include E'=E, the code sets g(X)=0 over the undefined range.

k) NEPTH, Number of energy points at which θ(E) is supplied. (NEPTH$\geq$2); FORMAT (I5)

l) (ET(L), θ(L), L=1,NEPTH); FORMAT (6E11.4),*L*N

Alternate energy, theta for this distribution. 3 pairs to a card. Energies increasing, spaced to permit linear interpolation for theta. For an incident E outside the θ-defining energy range, g(X) or dn/dE' is set equal to zero for all E', $0 \leq E' \leq E$.

m) (Supply only if LF=5; skip (m) and (n) if LF=9):

NPX, Number of values of X(=E'/θ) at which g(X) is supplied (NPX$\geq$2); FORMAT (I5)

n) (X(L), g(L), L=1, NPX) ; FORMAT (6E11.4),*L*N

Alternate X, g(X) for this distribution. 3 pairs to a card. Increasing X. At any E' with X=E'/θ(E) outside the tabulated range, g(X) is taken to be zero. Linear interpolation of g(X) in X is assumed.

Repeat items h-l (LF=9) or h-n (LF=5) for each subsequent distribution 2,...,NK.

Repeat items e-n for each subsequent reaction KREAC=2,...,NREAC.

End of type 7 input.

Item 4.8 - Type 8, Cross Section for Level Excitation

Here the individual cross sections for selected levels of a particular element are specified, as functions of energy on a single energy mesh for the perturbation.

Input:

a) KK,NES,ID,EL,EH; FORMAT (X,I4,I5,I10,2E15.5),*N

Perturbation index, Maximum number of energies at which σ-levels are given, element identification, perturbation E-low, E-high; NES≥2.

b) NLEVP, the number of levels perturbed (1≤NLEVP≤100);

FORMAT (I5)

c) (KLEV(K), NEL(K), K=1, NLEVP); FORMAT (16I5)

KLEV(K) is the level number of the Kth level perturbed;

NEL(K) is the number of consecutive energies in the input descending-energy mesh (item (d), below) at which the cross section for level KLEV is supplied (from the first (highest) energy downward). Alternate KLEV, NEL, 8 pairs to a card.

NOTE: 1. The KLEV's must be increasing, but need not be consecutive integers,

2. The first NEL must be ≤NES,

3. The NEL's must be non-increasing, and

4. The minimum value of NEL must be ≥2.

If these conditions are not satisfied by the data, the problem stops. A cross section must be defined for at least two energies since outside the range of energies for a cross section, the perturbation is taken to be non-existent, i.e., interpolation is not done between a perturbed and an unperturbed cross section.

d) E(L), L=1, NES; FORMAT (7E11.4),P*N

energies at which level cross sections are specified; in decreasing order; E(1)$\geq$EH for this perturbation, and E(NES)$\leq$EL.

The energy mesh should be chosen so that for any perturbation level, the cross section can be supplied for at least 2 energies, and such that linear interpolation in energy is correct.

e) For each perturbed level, supply

σ_{ℓ}(J),J=1, NEL(K); FORMAT (7E11.4);P*N

Cross Sections corresponding respectively to the first (highest) NEL(K) energies of the list (d). 7 to a card.

Start a new card for each new level. If scaling is used, one must enter P*N for the first card of each new level. Scaling may differ from level to level.

Item 4.9 - Type 9, Angular Distribution of Discrete-Level Inelastic Scattering

The first portion of the data required (items (a)-(d)) is the same as for type-8 input; restrictions on the NEL(K) are less stringent.

Input:

a) KK,NES,ID,EL,EH; FORMAT (X,I4,I5,I10,2E15.5),*N

NES = number of energies at which (μ,dp/dμ) tables are given for selected levels; NES$\geq$2.

b) NLEVP, number of levels perturbed (1$\leq$NLEVP$\leq$100); FORMAT (I5)

c) (KLEV(K), NEL(K), K=1, NLEVP); FORMAT (16I5)

KLEV(K) is the level number of the Kth level perturbed,

NEL(K) is the number of consecutive energies in the input descending-energy mesh (item (d)) at which angular-distribution tables (μ,dp/dμ) for level KLEV is supplied, from the first (highest) energy downward.

8 pairs to a card.

NOTE: 1. the KLEV's must be increasing, but need not be consecutive integers,

2. $2 \leq NEL(K) \leq NES$, and

3. the NEL's are not otherwise constrained.

d) E(L), L=1, NES; FORMAT (7E11.4), P*N

energies at which angular-distribution tables are specified; in decreasing order; $E(1) \geq EH$, and $E(NES) \leq EL$. The energies should be close enough to permit linear energy interpolation for $dp/d\mu$ at a given μ.

For each perturbed level, supply items (e):

e) Within this level, supply e.1, e.2 for NEL (level) energies.

(e.1) NMUP(≥ 2); FORMAT (I5)

No. of $(\mu, dp/d\mu) = (\cos\theta_{c.m.}, dp/d\mu)$ pairs supplied over range $-1 \leq \mu \leq +1$

(e.2) $\mu(L)$, $dp/d\mu$ (L), L=1, NMUP; FORMAT (6E11.4),*L*N

Three pairs to a card. The first $dp/d\mu$ should correspond to $\mu=-1$, the last to $\mu=+1$; (the code sets $\mu(1)=-1$ and $\mu(NMUP)=+1$). The values of $dp/d\mu$ should correctly represent the shape of the desired distribution but they need not be normalized; this is done by the code so that $\int_{-1}^{1} \frac{dp}{d\mu} \, d\mu = 1$. Linear interpolability of $dp/d\mu$ in μ is assumed.

(Supply e.1, e.2 for all energies E_1 (highest) to E_{NEL} for this level.)

(Repeat package (e.1, e.2) x NEL_{level} for each successive perturbed level.)

End of type-9 input.

Item 4.10 - Type 10, Source Spectrum

Input:

a) KK,NES; FORMAT (X,I4,I5)

Pert. index; No. of energy-boundaries specified for source-spectrum histogram (NES$\geq$2).

b) (E(L), S(L), L=1, NES); FORMAT (6E11.4), *L*N

NES pairs of (Energy, $\Delta S/\Delta E$); energies increasing;

E(1)$\leq$EELOW of entire problem (first card of input), and

E(NES)$\geq$EEHIGH. The source density $S(L)=\frac{\Delta S}{\Delta E}$ represents the constant value referring to the range from E(L) to E(L+1); hence S(NES-1) is the last pertinent value of S read.

This concludes the perturbation-data input. The following section gives a resume of the input and formats.

3.3 Summary of Input Data for Program SAMIN

	DATA and Restrictions	FORMATS
Item 1.	EELOW, EEHIGH, ISSW(1,2,...,12) Energy limits for tracking, and sense switch options	(2E11.4,8X,12I1),*N
Item 2.	NTYP(1,2,...,10) NTYP(K)=number of perturbations of type K present in the data. (If all are zero, end of input). Otherwise:	(10I5)
Item 3.	For each perturbation: KK,NPROB, (JPROB(L), L=1,NPROB) KK=pert. no., NPROB=no. of affected problems ($\leq$10); JPROB(1,2,...,NPROB) are distinct numbers, each $\leq$10. NPROB may be zero; if it is, data for pert. KK is subsequently limited to 1 card (that with item KK in columns 2-5).	(12I5)
	Data for specific perturbations with KK=1,2,..., $\sum_{L=1}^{10}$ NTYP(L):	
Item 4.1 - Type-1, Composition		
a)	KK, ICOMP, NLM Pert., composition no.,no. of elements	(X,I4,2I5)
b)	CONC (1,2,...,NLM) Concentrations (atoms/barn-cm)	(7E11.4),P*N
Item 4.2 - Type 2, Whole Element		
a)	KK, ID1, ID2 Pert., base ID, perturbing ID.	(X,I4,2I10)

Items 4.3-4.5 - Types 3,4,5 ($\sigma_t, \sigma_s, \sigma_{in}$)

a) KK, NEP, ID, EL, EH, FMULT (X,I4,I5,I10,3E15.5),*N

Pert., no. of energy pts., element ID, E-low, E-high, multiplier for X-sects (used if NEP<2).

b) (omit b if NEP<2)

If NEP≥2:

(E,σ) for L=1,2,...,NEP (6E11.4),*L*N

(Energy (eV), cross section (barns)) pairs, three to a card. Energies increasing, must span EL and EH.

Item 4.6 - Type 6, Angular Distribution of Elastic Scattering

a) KK, NE, ID, EL, EH (X,I4,I5,I10,2E15.5),*N

Pert., energies for distributions, element ID, E-low, E-high

(NE≥2)

b) E(1,2,...,NE) (7E11.4),P*N

Energies (eV, increasing); must span EL, EH.

c)-(e): CHI-table criteria:

LADHOC(≤40), N(≤50) (2I5)

Max. no. of CHI boundaries, No. of moments to compare

If LADHOC=0, skip (d) and (e); (go to (f))

If LADHOC≥1, and if N=0, skip to (e); (if N>0, go to (d))

d) $\varepsilon(1,2,\ldots,N)$ (10F8.3)

Allowable deviations in N moments past the zero-th

e) α (E12.4)

Allowable fractional deviation of χ-table ($dp/d\mu$) for bin-maximum $dp/d\mu$ tabulated

f) LTT = 1: Legendre coefficients supplied, or

2: Tabulated μ, $dp/d\mu$ supplied (I2)

Next supply (g), (h) if LTT=1 or (i), (j) if LTT=2:

(LTT=1): (g) NL ($\leq$50) (I5)

No. of Legendre coefficients supplied (omitting zero-th)

(h) C(1,2,...,NL, Legendre (7E11.4)

coefficients of normalized C.M. angular distribution.

(Repeat (g), (h) for each subsequent energy)

or

(LTT=2): (i) MNP ($2 \leq MNP \leq 100$) (I5)

No. of (μ,$dp/d\mu$) pairs supplied

j) (μ,$dp/d\mu$) (MNP pairs) (6E11.4)

First and last $dp/d\mu$ should correspond to μ=-1. and μ=+1. respectively; center-of-mass distribution, not necessarily normalized.

(Repeat (i), (j) for each subsequent energy).

Item 4.7 - Type 7, Secondary-Energy Distribution of Inelastic Continuum

a) KK,NES,ID,EL,EH (X,I4,I5,I10,2E15.5),*N

NES= No. of energies at which energy distribution data are supplied; ($\geq$2)

b) NENN (1,2,...,NES) (16I5)

No. of ENN boundaries for each incoming energy. Should be an increasing sequence; NENN(1)$\geq$2.

(Code corrects sequence if necessary.)

c) E(1,2,...,NES) (7E11.4),P*N

Incoming energies (eV) increasing; must span EL, EH

d) NREAC ($\geq$1) (I5)

No. of reactions contributing to inelastic continuum. Supply items (e)-(n) for each reaction present:

e) KREAC, MT, NK (X,I4,2I5)

Reaction no., reaction type, no. of distributions for this reaction. MT must have one of the values listed:

MT	Meaning
4	(n,n')
16	(n,2n)
17	(n,3n)
22	(n,n'α)
23	(n,n'3α)
24	(n,2nα)
25	(n,3nα)
28	(n,n'p)

f) NEPS ($\geq$2)

No. of energy points for reaction cross section

g) ($\underline{E}$,$\underline{\sigma_k}$), NEPS pairs (6E11.4),*L*N

(Increasing energies); σ_k assumed zero outside of defining range of E.

Within this reaction, supply items (h)-(l) or (h)-(n) for each of the NK distributions.

h) NEPP ($\geq$2) (I5)

No. of energies for p of distribution.

i) ($\underline{E}$,$\underline{p}$), NEPP pairs (6E11.4),*L*N

(Increasing energies)

j) LF,$\underline{U}$ (I5,E15.4),*N

LF=5 (X,g(X)) or 9 (Maxwellian);

U is used if LF=9; U$\geq$0.

k) NEPTH ($\geq$2) (I5)

No. of energy points for θ.

l) ($\underline{E}$,$\underline{\theta}$), NEPTH pairs, (6E11.4),*L*N

Energies increasing.

m) (Supply only if LF=5; skip (m) and (n) if LF=9)

NPX ($\geq$2) (I5)

No. of X points for g(X)

n) ($\underline{X}$,$\underline{g(X)}$), NPX pairs (6E11.4),*L*N

Increasing X.

Repeat h-l (if LF=9) or h-n (if LF=5) for each subsequent distribution within a reaction. Repeat items e-n for each subsequent reaction.

Item 4.8 - Type 8, Cross Section for Level Excitation

a) KK, NES, ID, EL, EH (X,I4,I5,I10,2E15.5),*N

NES=no. of energies for σ_{level}; ($\geq$2).

b) NLEVP (1$\leq$NLEVP$\leq$100) (I5)

No. of perturbed levels:

c) (KLEV(K), NEL(K), (NLEVP pairs) (16I5)

KLEV=level no., increasing; not necessarily consecutive numbers.

NEL=no. of energies (from highest down) at which σ level is given;

$2 \leq NEL(K) \leq NES; \quad \frac{d(NEL(K))}{dK} \leq 0.$

d) E(1,2,...,NES) (7E11.4),P*N

Energies for cross sections; decreasing order. Must span EH, EL.

e) For each of the NLEVP levels:

σ_ℓ(1,2,...,NEL(K)) (7E11.4),P*N

Values of σ level (barns) at E(1), E(2)...E(NEL(K)).

Start a new card for each level. If scaling is used, first card for each new level must have P*N desired for that level.

Item 4.9 - Type 9, Angular Distribution of Discrete-Level Scattering

a) KK, NES, ID, EL, EH (X,I4,I5,I10,2E15.5),*N

NES=no. of energies at which tables of $dp/d\mu$ are supplied ($\geq$2)

b) NLEVP (1$\leq$NLEVP$\leq$100) (I5)

No. of levels perturbed

c) (KLEV(K), NEL(K), (NLEVP pairs) (16I5)

NEL(K) is no. of energies at which tables of $(\mu, dp/d\mu)$ are supplied; KLEV's increasing; $2 \leq NEL(K) \leq NES$

d) E(1,2,...,NES) (7E11.4),P*N

Energies, decreasing, at which distribution tables are supplied, must span EH, EL.

For each perturbed level, supply e.1, e.2, repeated for NEL_{level} energies:

(e.1) NMUP (≥2) (I5)

No. of $(\mu, dp/d\mu)$ pairs

(e.2) $(\mu, dp/d\mu)$, (NMUP pairs) (6E11.4),*L*N

First and last μ's should be -1 and +1. $dp/d\mu$ may be un-normalized.

Repeat package (e.1, e.2) for all energies E(1),...,E(NEL(K)) for this level.

Repeat package (e.1,e.2) for all subsequent levels.

Item 4.10 - Type-10, Source Spectrum

a) KK, NES (X,I4,I5)

Pert., No. of energies (NES≥2).

b) (E,S(E)), NES pairs (6E11.4),*L*N

Energies increasing. Must span problem EELOW, EEHIGH.

S(1) is constant source density from E(1) to E(2), etc.

End of Input.

3.4 Tape Utilization

The following describes the function of each tape used in this program. Tape numbers refer to Fortran logical numbers. All tapes are used in the binary mode.

Tape 8

The processed perturbation data tape generated by program SAMIN to be read in by the next programs, SAMSAM and SAMCAR, as well as SAMGAM for a secondary γ problem.

Tape 12

A temporary storage tape used in subroutine FILE4P for construction of CHI-table.

Tape 14

A temporary storage tape used in subroutine FILE5P for construction of ENN-table.

Tape 15

A temporary storage tape used in subroutine FILE5P for construction of ENN-table.

4. PROGRAM SAMSAM: NEUTRON TRANSPORT PRE-PROCESSOR

4.1 General Discussion

In Chapter 2, we discussed the fact that SAMCEP performs Monte Carlo samplings from sampling densities which are defined to be least upper bounds (l.u.b.), or renormalized l.u.b., of physical sampling densities appropriate to each of the correlated problems considered.

Most of these sampling densities are generated by the SAMCAR code, during the course of Monte Carlo, only as the need arises.

The exceptions are angular distribution and continuous energy distributions, for which the sampling tables are precomputed in the relevant energy ranges prior to the start of the Monte Carlo calculation.

The precalculation of these sampling tables is performed by the SAMSAM code, subsequent to the generation of a BAND tape.

The SAMSAM code accepts as input the unperturbed data in the form of a BAND tape, and the definition of perturbations, as specified by the output of the SAMIN program.

The sampling tables generated by SAMSAM are broken up into energy bands and the information is written on tape 12 in a format described in Appendix C.

A record is also added to tape 8 (SAMINP tape), consisting of KEGEOM and the INBAND array, where KEGEOM is the length of the largest cross section data band and INBAND is of dimension NBAND. INBAND (I) = 1 or 0 if any tables are present in, or missing from, the $I^{\underline{th}}$ band.

4.2 Methodology

Generally, the user of the program will have at his disposal an Element Data Tape (EDT, output tape of processor SAM-X) which contains, for every isotope in the problem, a set of energy-dependent interaction cross sections. The user must then specify each of the material compositions appearing in the problem. A composition is defined in terms of atomic concentrations, C_i, (in units

of 10^{24} atoms/cm^3) of each isotope, i, in the composition. These may be calculated from the expression:

$C_i = 10^{-24}$ x Avogadro's number x mass density/atomic weight. For compounds or mixtures the concentration of each component must be specified. In addition, each composition must be identified by a composition number.

This input is processed in conjunction with the EDT by the BAND routine, which generates an Organized Data Tape (ODT). The ODT contains all the elemental cross section data in energy band structure*. During the tracking process, the data retrieval (DR) routines of program SAMCAR will use this information to determine:

1. The probability that a particle has an interaction in a region of given composition,
2. The element with which the particle interacts,
3. The type of interaction (absorption, elastic scattering, etc.) occurring,
4. The energy and direction of the particle after interaction.

The sampling CHI- and ENN-tables of a specific element are tabulated at the energy mesh points of the unperturbed CHI- and ENN-tables of that element. If perturbation type 2 (entire element perturbed) is present, or the perturbation energy ranges overlap, there will be just one sampling table for that element in the affected energy band. Only if there is an energy gap in the basic energy mesh with no perturbations (type 2, 6 or 7), will there be separate sampling tables for the separate perturbation energy ranges in this energy band. At each energy mesh point, a sampling table is generated by subroutine NVLOPE according to the number of such perturbations affecting this energy. Together

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*The energy band structure may be user specified, or, optionally computed internally on the basis of available memory for cross section storage (i.e., automatic banding).

with the sampling tables written on tape are the perturbation ID's (i.e., IP's) so that we can fill in the location of sampling tables for each perturbation after the sampling tables are read into memory from tape during the execution of program SAMCAR.

SAMSAM first calls subroutine BAND to process the unperturbed element cross section data into energy bands and to store the processed data on tape. Subsequently, SAMSAM reads in the processed data, a band at a time, into the MASTER-array (refer to organization of the MASTER-array in Appendix B) and then fills the perturbed element locations into MISTER-array (refer to storage map description of MISTER-array in Appendix C). With both the perturbed and unperturbed element cross section data in memory, SAMSAM next calls subroutines SAMCHI and SAMENN to retrieve all perturbations of type 2, 6 or 7 in the current energy band, and to group such perturbations of the same element together. For each element, SAMCHI (or SAMENN) will call subroutine CHIA (or ENNA) to interpolate and tabulate the unperturbed and perturbed CHI- (or ENN-) distributions in the energy mesh of the unperturbed element's CHI- (or ENN-) table. CHIA (or ENNA) in turn calls subroutine NVLOPE to generate the sampling CHI- (or ENN-) table at the given energy mesh. The length of the sampling table is set at a constant value of 15 (including 0 and 1 in the case of CHI- table); this simplifies the logic of the program, and the chosen length is considered to be adequate for reasonable superpositions of angular or energy distributions.

It is possible that perturbations of type 6 and 7 (angular and secondary energy distribution) exist, yet no sampling table is generated. This is the case when the perturbation energy range (EH and EL) falls within two energy mesh points of the basic energy table.

4.3 Description of Input Data for Program SAMSAM

Item 1 - IODT = 0 or KEGEOM (Format I5)

IODT = 0, SAMSAM will call subroutine BAND to process element data tape (output tape of SAM-X);

IODT = KEGEOM, the call to BAND is bypassed.

KEGEOM is the total length for all the element data, as computed (and displayed) by a call to BAND in a previous execution of SAMSAM.

Item 2 - NBAND = total number of energy bands supplied* (Format I5)

or NBAND = 0 effects the automatic banding option.

The user supplied value determines the input items to be supplied next:

If NBAND = 0, supply Items 3a and omit 3b.

If NBAND>0, omit Items 3a and supply 3b.

Items 3a - automatic banding input (NBAND=0)

Card #1 - EX1, EXLAST (Format 2E11.4)

high, low cross section energy limits**;

Card #2 - NROOM, NEL (Format 2I5)

where NROOM is the number of words of memory available for the longest BAND of data (internally set to 5000 if left blank); and NEL is the number of different elements in the present calculation;

Card(s) #3 - ID(I), I=1,NEL (Format 16I5)

complete list of element ID's (ZZAAA) in any order;

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* Currently limted to 19.

** See Appendix H.

Item 3b - user specified banding (NBAND>0)

EBAND(I),I=1, (NBAND+1); energy band limits.

(Format 7E11.4)

Enter the energy limits (in ev) of each band starting with the highest energy and proceeding to the lowest energy in the problem*. Use as many cards as necessary.

End of data if IODT=KEGEOM.

If IODT=0, continue with next items.

Item 4 - Composition Identification (Format 7I10)

NO = Problem number - identification of present run.

NCOMP = Composition number - total number of compositions in the problem.

NG = 0 for neutron transport problem.

Item 5 - NE - Number of elements (Format I10)

Enter the number of discrete nuclides.

Item 6 - Element cards (one card for each of the NE elements)

(Format 2I10, E15.6)

IT - blank

ID - an integer which identifies each element.

(Five decimal digits: ZZAAA)

Concentration - enter the atomic concentration (10^{24} atoms/cm^3 of this element in the composition)

Items 5 and 6 are repeated for each composition.

End of data for program SAMSAM.

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* See Appendix H

4.4 Tape Utilization

The following describes the function of each tape used in this program. Tape numbers refer to Fortran logical numbers. All tapes are used in the binary mode.

Tape 8

The processed perturbation data tape, output of program SAMIN. Data on this tape is modified and expanded by SAMSAM*. This tape will be read in by next program SAMCAR, and, subsequently, by SAMGAM, if a secondary γ problem is being solved.

Tape 9

A temporary storage tape is used by subroutine BAND if NBAND > 1.**

Tape 10

The organized data tape, output tape of BAND with cross section data in band structure.

Tape 11

The neutron element data tape, output tape of processor SAM-X which contains a library of element data including, at least, all elements required for the problem being run. Subroutine BAND reads in this tape to process its data into energy band structures.

Tape 12

This tape is generated by program SAMSAM. It contains the sampling CHI- and/or ENN-table in the same band structure as the unperturbed data. This tape will be read in by the next program SAMCAR if perturbations of this type are present.

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* Number of bands and energy band limits are appended by SAMSAM, to be read in by SAMCAR (maximum number bands currently 19.)

** Although NBAND is set to zero (by the user) to invoke automatic banding, it is internally reset to correspond to the number of computed BAND intervals.

5. PROGRAM SAMCAR: NEUTRON AND SECONDARY GAMMA CORRELATED MONTE CARLO TRANSPORT CODE

5.1 General Discussion

SAMCAR is the main correlated Monte Carlo program which calculates the transport of particles* through matter (both time-dependent or time-independent) with correlated sampling techniques. It is composed of a series of independent routines which perform the following three basic functions:

1. Process geometry data by calling GENI.
2. Process the unperturbed and perturbed source spectrum by calling subroutine SOUCAL**.
3. Perform the transport calculations and score the particle fluxes by calling subroutine CARLO. SAMCAR writes the particle fluxes by supergroups of all problems (unperturbed and perturbed) by statistical aggregates on tape to be edited by the next program SAMOUT.

Basically, the program requires as input a geometry specification, the elemental composition of each region, and a specification of the location and time-, energy-, angular distributions of the radiation source**. The program selects individual particles from the given source distribution*** and tracks them through a series of interactions within the geometry until such time as the particle history is terminated. The tracking of a particle can be terminated for any of the following reasons:

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* neutrons and secondary gamma rays.

** for primary neutron problems.

*** or external source tape, for secondary γ problems.

1. The energy of the particle after an interaction falls below a specified 'cutoff energy'.

2. The time variable of the particle exceeds a specified 'cutoff time'.

3. The particle escapes from the geometry (crosses an external boundary).

4. The particle is 'killed'. This procedure will be explained in the section dealing with the importance sampling techniques employed in the program.

For each scoring region* traversed by a given particle, the code computes the flux per unit time per unit energy as a function of energy and time for each problem. The flux contribution for a given particle is defined as its expected total path length contribution in a region divided by the volume of the region. Individual particle flux contributions are accumulated so that the end result of the tracking process is the total flux in each region in a specified group of energy and time bins. At the user's option the problem can be made time independent.

The above description of the SAMCAR program is, of course, a very simplified view of the computational procedure. The following sections provide a more detailed, although non-mathematical, description of each part of the computation.

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* Refer to Sections 5.2.1 and 5.2.9.

5.2 Input Requirements

5.2.1 Bounded Point Detectors; Region Terminology

With the inclusion of bounded-flux-at-a-point (BFAP) estimation, the concept of a scoring region has been generalized to include point detectors. This generalization has necessitated an expansion of "region" terminology with the introduction of two qualifiers: physical and material. Thus, a point detector is located within a "physical" region; its flux estimates are scored in an input designated "scoring" region; and its sphere of influence* is determined from the element concentrations in its designated "material" region, or, as a user input option, given explicitly.

For each detector, the user specifies a coordinate location, scoring region, and material region. The detector's physical region is internally determined from its position coordinates. If the material region is unspecified, the default material region is the physical region. If a negative value for the material region is specified, the critical radius is given explicitly**.

Note that any physical region may itself be designated as a scoring region, and the element concentrations of any physical region (scoring, non-scoring, or even the escape region, which may comprise a "phony" material) can serve as the designated material region for any detector.

In the sections that follow, the generic term "region" will refer to a physical region, where the specific reference is clear from context. Also, whenever applicable, references to scoring regions are equally valid for point detectors.

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* Refer to Sec. E.3.1 of Appendix E.

** Refer to Item 10 of Sec. 5.3.

5.2.2 Geometry Input

The specification of the geometry and its input format is described in Appendix A of this report. It makes use of the Combinatorial Geometry Technique. The geometry data must be prepared in units of centimeters to be consistent with the cross section data.

5.2.3 Importance Sampling

A. General

Importance sampling or 'weighting' provides the user with a powerful method of controlling the direction and/or energy of particles in the problem. The purpose of a particular problem, for example, may be to calculate the fast-neutron flux in a given region within the geometry. Under normal circumstances, the probability of a source neutron reaching that region at high energy may be quite small, requiring a vast number of source neutrons to be tracked before an adequate statistical estimate of the flux is obtained. However, with proper particle weighting the code can be made to concentrate only on those fast neutrons having the best chance of reaching the chosen region. Conversely, the code will spend little time tracking neutrons which are either traveling in the wrong direction or are at relatively low energy.

The program determines the relative importance of a particle from a parameter called the weight. The total weight (W) of a particle is, in turn, determined from a combination of three quantities called region weight (W_R), angular weight (W_Ω), and energy weight (W_E), where $W = W_R \times W_\Omega \times W_E$. Values of W_R, W_Ω, and W_E are given as input. The following brief discussion should provide the user with a better insight into how these weights are actually used by the code.

For the normal uncorrelated Monte Carlo problem, a quantity F is assigned to each particle. The value of F is 1.0 for a source particle. The code

calculates the probability that the particle will reach the boundary of the source region along its flight path without collision. This value is called F". The probability that a collision takes place in the region is then 1-F". However, in the case of a correlated problem, we would have instead N problems (unperturbed plus (N-1) perturbed problems). The value of F for each problem is normally 1.0 for a source particle. But when the source spectrum is perturbed (perturbation type 10) the sampling source spectrum is the envelope of all source spectra instead of any given source spectrum. F, therefore, is different for each problem, and in fact F=1.0 for the problem whose source spectrum happens to be the envelope and the rest will have a value of F<1.0 which is the ratio of a given spectrum over the envelope spectrum.

The probability that a collision takes place in the region is more complicated in the case of a correlated problem when the macroscopic total cross section is perturbed (perturbation type 1, 2 and 3). Here we do not sample from any particular distribution but we sample from the envelope of all distributions. The probability of having a collision at a distance S for the i^{th} problem is $F_i\mu_i e^{-\mu_i S}dS$, where μ_i= the macroscopic total cross section of the i^{th} problem, and the probability of not having a collision in the region is $F_i'' = F_i e^{-\mu_i Sl}$, where Sl is the distance to the region boundary. The sampling distribution for picking a collision position is the envelope of all $F_i\mu_i e^{-\mu_i S}$ for i=1 to N in a given region*. At collision, quantities F_i^C are calculated for the single collision event for each of the problems i, as the ratio of the i^{th} collision probability distribution function $F_i\mu_i e^{-\mu_i S}$ over the single sampling distribution. The collision mechanics and further adjustments to the F_i^C's will be discussed elsewhere (see section DR3). In any case, the particle coming out of collision and its adjusted F_i^C's are stored for later processing and

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* Bounded estimation procedure modifies this usage (refer to Sec. E.3.3 of Appendix E.)

do not affect the further tracking of the original particle. The further tracking of the original particle consists in attempting to generate further collisions in the same region, and when they, if any, are exhausted, to enter into the next region.

If the next region is the "escape region", the tracking of the particle terminates. If not, the entrance into the new region will modify the F_i's by the new region weight. Suppose that the source particle is leaving region 1 where the weight is W_1 and entering region 2 where the weight is W_2. At the boundary the ratio of weights W_1/W_2 is multiplied by F''_i's and the particle is given a starting value of $F_i=F''_i\ W_1/W_2$ in region 2. The probability of the particle reaching the next boundary of region 2 uncollided is calculated and multiplied by F_i for each problem to obtain a new value of F''_i. Notice that if W_2 is large compared to W_1, the probability is high that no latents* will be produced since both F_i and F''_i will be small compared to unity. In fact, a parameter F_z is an input to the program, and if the largest of these F_i's, on entry into a new region, is lower than F_z, a random number between zero and one is picked. If the number is greater than the largest F_i, the history is terminated. If it is lower than the largest F_i, the history is continued with all the F_i's divided by the largest F_i. Thus, by establishing weight sets properly, increased numbers of collisions can be forced to occur in important regions, and in addition, the original source particles will continue to propagate through the geometry.

Without going into detail, it can be stated that a small value of F_z minimizes the number of kills (increases problem running time). A large value maximizes the kills (decreases running time per history) but increases the

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* Refer to Section F in 5.2.3.

variance (or error) of the answers, requiring more source particles to be run. The optimum value of F_z will generally lie in the range from 0.01 to 0.1.

In order to facilitate input preparation, the three components of the total weight will now be discussed separately.

B. Region Weights

A region weight (W_R) must be specified for every region in the problem. Ordinarily, these weights are set up so that they gradually decrease as a particle proceeds from the source toward a region in which the flux is desired. Weights should gradually increase in regions which are located progressively further from the 'important' regions. On the input forms the user must specify all values of W_R to be used in the problem. The order in which these values are entered determines their region weight number (i.e., the first value of W_R is labelled weight #1, the second value is weight #2, etc.). Then for each region, the weight number to be used in that region must be specified.

C. Angular Weights

By using angular weighting, it is possible to specify preferred directions for a particle, independent of the region location of the particle. The user first specifies the direction cosines (with respect to the coordinate axes of the problem) of one or more aiming angles. These vectors serve as 'zero directions' about which angular weights will be given. Each aiming angle is assigned a number. Next, a set of angular bins is specified between 0° and 180°, with the bin boundaries given in terms of their cosines. Thus, if one desires to specify four bins of equal angle, the cosines of 0°, 45°, 90°, 135°, and 180° should be entered. Then, one or more sets of angular weight values are given. For each set, a weight value (W_Ω) is specified for each angular bin. Each set is also assigned a number. Finally, for each region, the aiming angle number and the angular weight set number must be given. To illustrate how the code uses this information, assume that a given region has been assigned aiming

angle #1 and angular weight set #2. A particle enters the region and the code determines that the particle is traveling at an angle Ω with respect to aiming angle #1. The code then determines which angular bin encompasses Ω, goes to angular weight set #2, and finds the value of W_Ω in that bin.

In general, as the particle direction (angular bin) becomes more important, the value of W_Ω assigned to that bin should decrease.

D. Energy Weighting

The use of energy weighting enables the user to instruct the code as to which particle energies are most important in a given problem. A set of energy bins is first given, where the bin boundaries are listed in decreasing order. Then, one or more energy weight sets are specified, with each set being assigned a number. For each set an energy weight value W_E must be given for each energy bin. The energy weight set number corresponding to each region is then given. Assume, for example, that a particle of energy E is in a region which has been assigned weight set #1. The code first locates the energy bin which encompasses E, refers to weight set #1, and determines the value of W_E which was given for that bin. In establishing the energy weights, the more important energies should generally have smaller W_E values than the less important energies.

E. Application of Weights to Tracking

As noted earlier, the total particle weight is the product of $W_R \times W_\Omega \times W_E$. The particle weight is used to determine the number of collisions that a particle will produce given that it has a specified energy and direction in a given physical region. By an appropriate choice of aiming angle and angular weights, particles heading downward can be caused to have more collisions than particles heading upward in the same region. Thus, more computing time will be spent on the 'important' downward-directed particles and their descendents than on the 'less important' upward-directed particles.

F. Treatment of 'Latent' Particles

If a collision does occur, the program calculates the energy and direction of the particle emerging from the collision. The collided particle is stored in a latent storage table together with the N values of F_i^C (refer to section A of 5.2.3), and will be picked up and followed as though it were a source particle at a later time. When it is started out as a real particle, it is assigned a new F_i value for each problem which is the product of F_i^C and the ratio of the weight (product of region, energy and angular weights) before and after collision. In general, the new F_i's will be different due to differences in energy and direction of flight if energy and angular importances are present.

The program stores the information concerning latents in a table which can hold up to 100 latents. Prior to storage a test is made to see if the largest F_i of the latent exceeds the input value of F_z. If so, it is stored. If not, a game of Russian roulette is performed, as previously discussed, and the latent is either eliminated or has its F_i's renormalized by dividing all of them by the largest F_i.

If more than 100 latents are generated by a source particle, the program has a 'squeeze' routine which reduces the number of latents in a statistically valid way.

Although the use of importance sampling may appear to be a rather complicated procedure, the user will generally find that after gaining a little experience with the code the process becomes relatively straightforward and easily applied. Certainly, the time spent in learning how to properly apply this technique will be well worth it in the long run, since it enables complex, deep-penetration problems to be run in a reasonable amount of machine time.

5.2.4 Source Specification

The specification of the initial particle source provides the user with several options. These options are described briefly below.

5.2.4.1 Internally Generated Primary Neutron Source

Perturbation of the source is allowed only in changing the shape of the source spectrum itself, and the input of the unperturbed and perturbed spectra must be in the form of histograms.

A. Spatial Distribution

Sources may be generated in any number of regions, but the region must be single bodies and restricted to SPH, RCC, BOX, RPP, TRC. For each source region the 'power density' (particles/volume) must be given. The user has the option of normalizing the problem to a unit source or to the total input power.

B. Angular Distribution

Sources may be either isotropic or monodirectional but the same angular distribution must be used in all source regions. (It should be noted, however, that a source may be generated in a finite cone by specifying an isotropic distribution and using angular weights to kill particles which are generated outside the desired cone.)

C. Energy Distribution

The source energy spectrum is specified by a histogram. The input of the source energy spectrum contains the desired energy mesh E_i's and the height of the histogram in interval E_i to E_{i+1} (i.e., a table of E vs. S(E) is required).

D. Time Distribution

If a time-dependent problem is to be run, the user must supply a table of time values and the integrated source up to each time (i.e., t vs $\int_0^t S(t)dt$). This input should be deleted from time-independent problems.

5.2.4.2 Secondary Gamma Source from Previously Generated Interaction Tape

Using a neutron interaction tape (see Section 5.2.12), and gamma ray production data supplied by SAM-X, SAMGAM can generate, internally, sources of secondary gamma radiation. Note that the interaction tape must have been generated by a precursor primary neutron SAMCAR calculation. A detailed description of Program SAMGAM is given in Chapter 7.

5.2.5 Time Dependence

SAMCEP enables the user to compute particle fluxes as a function of time as well as energy and position. The user selects any desired time bin structure for the problem and enters the bin limits in consecutive order on the input forms, starting with the latest time. Output fluxes will be given in this bin structure in the edit. During the tracking process the code computes the flight time of a particle between collision points from its velocity (or energy). Interactions are assumed to occur instantaneously. By accumulating the flight times for each particle, the code is capable of storing particle fluxes in the proper output time bins.

5.2.6 Output Energy Mesh; Supergroups and Superbins

During tracking, the code stores fluxes in each region in a set of energy output bins specified by the user. The number and width of these bins are arbitrary. The bin limits must be given consecutively in the input, starting with the highest energy. The upper and lower bin limits must be preceded by minus signs. The reason for this will be explained shortly. Care should be taken to insure that the upper energy bin limit is equal to or greater than the highest source energy to be generated in the problem. A cutoff energy is also specified, which instructs the code to cease tracking any particle which degrades below this energy. The user should be certain that the lowest energy bin limit is equal to or lower than the cutoff energy. In essence, there must be a bin available to store every possible energy in the problem.

Some calculations may require more computer storage than is available. This situation can be alleviated by using the 'superbin' option provided by the code. This option divides the overall output energy range into smaller groups (called supergroups) and the cross section energy range into bands. The intersection of band and supergroup defines a superbin. The code then treats each of these superbins separately. In this manner, only the cross section data for the band currently being treated are stored in the memory; only fluxes for the supergroup currently in memory are scored; and only those particles having energies in the corresponding superbin are tracked. When a particle degrades to a lower bin, its parameters are stored and its tracking is resumed only after all higher superbins have been completed. The output supergroup structure is defined by the user by placing a minus sign before those output energies he wishes to designate as supergroup limits. If this option is not desired, only the upper and lower energy bin limits require minus signs. This instructs the code to treat all output energies as part of a single supergroup.

5.2.7 Response Functions

SAMCEP provides response function options which allow the user to automatically transform particle fluxes into any desired flux-dependent quantity (dose, heat deposition, etc.). Assume, for example, that the dose is required in several regions. The user supplies, as input in the next edit program, SAMOUT, a flux-to-dose conversion factor as a function of energy. For each region, SAMOUT multiplies the flux $\phi(E)$ in each energy bin by the corresponding conversion factor $D(E)$ and integrates over energy. Thus,

$$\text{DOSE} = \int_0^{\text{EMAX}} \phi(E) \times C(E) \times dE$$

5.2.8 Transmission* and Escape Regions

A transmission region has the property such that when a particle enters it, the tracking of that particle is continued but all of its parameters (X,Y,Z coordinates, energy, etc.) are stored on a magnetic tape called the interaction tape**. This tape then can be used to generate a source tape composed of particles entering the transmission region. In general, a transmission region is used when it is desired to run a problem in two steps. This is usually done for very deep penetrations or for unusual geometric configurations (such as ducts) where it may be more economical to run the problem in stages. The designation of a transmission region is, however, optional. Note that the program is capable of treating up to 10 different transmission regions.

An escape region is one in which all particles that enter are killed. It is ordinarily used to define the outer limits of the geometry (i.e., the complete geometry is enclosed in a large region which is designated as the escape region).

5.2.9 Scoring Regions

A scoring region is one in which the flux contribution is computed for each particle which passes through it***. In a non-scoring region no such computation is made, so that the output edit provides fluxes only in those regions designated in the input as scoring regions.

In most problems it is desired to know the flux in every region separately, in which case each region in the problem would be defined as a scoring region with a different number. In some problems, however, two or more regions may be completely symmetric with respect to the source, in which case the fluxes in these symmetric regions could be combined without any loss of information, and

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* Not applicable for point detectors.

** See Section 5.2.12

*** Recall that this concept has been generalized to include point detectors. (See Section 5.2.1)

in fact, an improvement in the accuracy will be obtained. Each of these regions then would be designated by the same scoring region number. In still other problems it may be unnecessary to know the fluxes in certain regions. These should then be given scoring region number zero, which tabs them as non-scoring.

Since fluxes are only stored and printed out for scoring regions, it is possible to reduce both the size of the edit and the core storage requirements by reducing the number of different scoring regions. It should be remembered, however, that once a problem is run it is impossible to recapture any flux information in nonscoring regions.

5.2.10 Number of Histories and Statistical Groups

The user must designate the total number of source particles (histories) to be run in the problem. Although a greater number of histories will improve the accuracy of the answers, it will also increase the problem running time. The user must, therefore, strike a balance between the tolerable errors in the answers and the cost of running the problem. In complicated problems it is usually wise to run a test problem of 100 to 200 histories to get a 'feel' for whether particles are reaching the desired regions. If they are not, the fault probably lies in incorrect importance sampling and the weights should be adjusted. If the test problem appears to have run 'well', then the number of histories can be increased by perhaps a factor of about 10. After some experience, the user can generally determine the correct number of histories to run in a particular problem.

In running the problem the total number of histories is divided into aggregates called statistical groups. This is done in order to compute the variance (or standard deviation) of the fluxes. All particles (and their latents) within a group are tracked before another group of particles. Fluxes are computed and stored on tape separately for each group. The size of the statistical group is

constant in a given problem and must be specified in the input. The group size is not critical but should be small compared to the total number of histories to be run. About 20 statistical groups per problem generally have been found to be adequate.

5.2.11 Volume Computations

To evaluate the flux, the track length in a region is divided by the volume of the region*. Provision has been made to input volumes of regions if they are known. It often happens, however, that regions described by the Combinatorial Geometry technique have such complex shapes that an analytic volume computation is not practical. To determine the volume of such regions, a routine is included to perform a ray-tracing numerical integration calculation of the volume.

A point $\bar{X}$ within the geometry is given as input. Rays are fired isotropically from the point $\bar{X}$ and the volume of each region is then

$$V_i = \frac{4}{3}\pi \sum \frac{(R_2^3 - R_1^3)}{H}$$

where R_1 and R_2 are the distances along the ray to the entrance and exit contacts with region i. 'H' is the total number of rays fired.

5.2.12 Interaction File

SAMCAR provides the user with a method of calculating the production and transport of secondary gamma rays arising from neutron capture or inelastic scattering events.

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* The flux estimates scored at point detectors are dimensionally equivalent to track length per unit volume.

During the tracking of primary source neutrons, all interactions which are capable of producing secondaries can be stored, as an option, on an "interaction" file. Among the stored data are the coordinates of the collision point, the energy and weight of the primary neutron multiplied by the non-elastic interaction probability, and the time of interaction. Subsequently, this file can be processed internally by SAMGAM and be converted into a source of secondary gamma radiation.

The interaction file can contain both interaction and transmission information. The 14th parameter of each particle record indicates the type of event.

5.3 Card Input Formats

Definitions of all input quantities and corresponding card formats are given below. The definitions are given in the order in which the data is required by the code.

Item 1 - Edit Title Card (Format 20A4)

This title will be printed by the next edit program, SAMOUT.

Item 2 - Debug Switches SSDR1, SSDR3 (Format 2I1)

SSDR1 = 1, debug printout from subroutine DR1.

= 0, no debug printout.

SSDR3 = 1, debug printout from subroutine DR3.

= 0, no debug printout.

Item 3 - Identification Card (Format 2I1, 3X, A3, 18A4)

IDBG = 1, debug printout for tracking of particle.

= 0, no debug printout.

IODT = 1, do not call BAND*.

NAME = identification of present SAMCAR run.

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*The output of a previously run BAND in SAMSAM or SAMGAM must be available and designated as Tape 10.

Item 4 - LRN = Random Number Initiator (Format 5X,I15)

If blank, the default option, (=1), will be used.

Code insures that LRN is positive, odd, and satisfies the condition: (1.LE.LRN.LE.2(48)-1).

Item 5 - LDUMMY - an arbitrary number (Format I10)

Item 6 - GENI (Geometry) Input

The Combinatorial Geometry (CG) input discussed in Appendix A must be preceded by a header card (Format I10, E15.4, A3, 13A4).

IPRINT = 0, print out body and region data which follow

= 1, print out body and region data as well as the internal arrays in which they are stored

= 2, suppress all geometry printout

SCALE multiply all CG dimensions by this scale factor (default = 1.0).

MA 45 arbitrary Hollerith characters

Item 7 - Statistical Data (Format 3I10, 8I5)

NSTART The number of real time seconds of running time before terminating and editing.

NSTOP Number of the last history to be treated.

NSTAT Number of histories per statistical group.

NRMAX Number of regions in the geometry.

NG — Enter 0 for a neutron problem, or 1 for a gamma problem.

NT — Number of output time bins (enter 0 for a time-independent problem).

NOUT — Number of output energy bins.

NUMSC — Number of flux scoring regions plus the number of detectors (as given in Item 9 below).

NRWL — Number of distinct region weights.

IREX — The escape region number.

IRT(1) — The first transmission region number (leave blank if no transmission regions are desired).

Note that the above 11 items appear on a single card, the first three are Format I10 and the last eight are Format I5.

Item 8 - Transmission-Interaction Information (Format 14I5)

IRT(2)

IRT(3)

IRT(4)

IRT(5) — Additional transmission region numbers.

IRT(6) — Leave blank if only one or if no trans-

IRT(7) — mission region, or if using point de-

IRT(8) — tectors.

IRT(9)

IRT(10)

IWE — Enter a '1' if elastics are to be recorded on tape, otherwise leave blank.

IWO — Enter a '1' if non-elastics are to be recorded on tape; otherwise leave blank.

Item 9 - Number of Point Detectors (Format I10)

NDET - Number of point detectors for which bounded statistical estimation will be used. If no detectors used, leave blank and omit next item.

Item 10 - Detector Coordinates, Scoring Region, "Material" Region, and (optionally) critical radius.

(Format 3E14.6, 2I5, E14.6)

Use one card for each of the NDET detectors (NDET>0).

XAD, YAD, ZAD - The X, Y, Z coordinates of the detector.

ISCA - The scoring region of the detector. A blank entry will suppress scoring for the detector. Otherwise, any number in the range (1,NUMSC), where NUMSC is specified in Item 7, is valid, but normally given as (NUMSC-NDET+1) through (NUMSC).

IRDET- The detector "material" region (if given >0). The radius of the detector's sphere of influence, i.e., "critical radius", is computed internally as the reciprocal of the sum of the concentrations of the elements in this specified region. A blank entry will assign the region in which the detector is located, as specified by its coordinates (i.e., its physical region). A negative entry implies critical radius specified by user as next entry on card.

CRAD - Critical radius (ignored if IRDET>0).

Item 11 - Cutoff Information (Format 2E14.5, 14X, 2E14.5)

ECUT — Low energy cutoff (ev). Tracking of a particle is terminated if its energy degrades below ECUT*.

ETH — Thermal energy if a thermal group is required. ETH must be within the energy limits of the problem.

FZ — See discussion in Section 5.2.3.

EHIGH — High energy cutoff (ev). This should be less than or equal to the highest energy for which cross sections are available*.

Item 12 - Output Energy Bins (Format 5E14.5)

These cards give the boundaries of the output energy bins (ev) used for the flux edit*. There should be five entries per card with a total of (NOUT+1) entries. The energies should be listed from high to low with the lowest energy equal to or less than ECUT. The first and last entries should be negative. If supergroups are used, any number of intermediate energies may also be negative. The absolute value of the highest output bin boundary must be >EHIGH.

Item 13 - Output Time Bins (Format 5E14.5)

These cards give the boundaries of the output time bins. There should be five entries per card with a total of (NT+1) entries. However, if NT=0, omit Item 13 entirely. Times should be entered from high to low and the last entry must equal 0. The first entry defines TCUT, the time cutoff.

Item 14 - Region Weights (Format 5E14.5)

These cards give all of the region weights needed in the problem. They are entered five to a card with a total of NRWL entries. The weights need not be entered monotonically by value, but their order determines the region weight numbers (i.e., entry one is weight #1, etc.).

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* See Appendix H.

Item 15 - Region Specifications (Format 6I5)

Use one card per region with a total of NRMAX cards. The first card applies to region 1, the second to region 2, etc.

ISC — Scoring region number in which the fluxes in this physical region are to be stored. Several regions may be assigned the same ISC number. If ISC=0, fluxes will not be scored.

NREG — Number of the composition to be found in this region.

IRW — Region weight number assigned to this region. A weight number is given by its position in the list of region weights.

IEW — Energy weight set number assigned to this region. If IEW=0, there is no energy weighting in this region.

IAN — Aiming angle number assigned to this region. If IAN=0, there is no angular weighting in this region.

IANG — Angular weight set number assigned to this region.

Item 16 - Energy Weight Specification (Format 2I10)

NEWL — Number of energy bins for energy weighting.

NEW — Number of distinct energy weight sets. If NEWL and NEW=0, the problem contains no energy weighting and Items 17 and 18 are omitted.

Item 17 - Bin Limits for Energy Weights (Format 5E14.5)

Enter the boundaries (ev) of the energy bins to be used for energy weighting*. There should be five entries per card with a total of (NEWL+1) entries. The energies should be entered in decreasing order. The lowest bin limit should be less than or equal to ECUT.

*See Appendix H

Item 18 - Energy Weight Sets (Format 5E14.5)

The energy weight value in each of the above energy bins should be entered. One or more sets of energy weights may be entered. Each set should contain NEWL entries and a new card should be used to start each set. There should be a total of NEW sets. The order in which the sets are entered determines the energy weight set numbers (the first set is weight set #1, etc.).

NOTE - Omit items 17 and 18 if no energy weighting.

Item 19 - Angular Weight Specifications (Format 3I10)

NAIML Number of distinct aiming angles.

NUMANL Number of angular bins for angular weighting.

NUMANG Number of distinct angular weight sets.

If the problem contains no angular weighting, enter 0 for the above three quantities and omit Items 20, 21 and 22.

Item 20 - Aiming Directions (Format 3E14.5)

Enter the direction cosines of each aiming angle with respect to the X, Y, Z coordinates. Use a total of NAIML cards.

Item 21 - Bin Limits for Angular Weights (Format 5E14.5)

Enter the boundaries of the angular bins to be used for angular weighting. Boundaries are given in terms of the cosines of the angles between aiming direction and particle direction, with the first entry equal to 1.0 and the last entry equal to -1.0. There would be a total of (NUMANL+1) entries.

Item 22 - Angular Weight Sets (Format 5E14.5)

The angular weight value in each of the above angular bins should be entered. One or more sets of angular weights should be entered. Each set should contain NUMANL entries and a new card should be used to start each set. There should be a total of NUMANG sets. The order in which the sets are entered determines the angular weight set numbers.

NOTE - Omit Items 20, 21 and 22 if no angular weighting.

Item 23 - Source Specifications (Format 3I10)

NSR — Number of different source regions in the problem. If NSR=0, an external source tape is used and no further source input is required (i.e., omit Items 24-28).

IFLAG — Number of energies used to define the source spectrum.

ISW — If ISW=0, fluxes will normalize to one source particle. If ISW=1, fluxes will be normalized to the total source power as implied by Item 24.

Item 24 - Source Regions (Format I10, E20.8, I10)

One card is required for each source region with a total of NSR such cards.

ISR — Geometrical region number.

P — Power density in the region (source particles per unit volume).

ISO — If ISO=0, the source will be emitted isotropically. If ISO=1, the source will be monodirectional, with the direction specified on Item 28. The value of ISO (0 or 1) must be the same for all source regions.

NOTE: Only single body source regions are allowed. Moreover, the choice of bodies is restricted to the following:

SPH, RCC, BOX, RPP.

Item 25 - Spectrum Description (Format 2E20.8)

These cards give the histogram of the source spectrum. Each card contains an energy (ev) and the height of the histogram to the right of the energy E. The first card contains the lowest energy, and the last card gives the highest energy of the source*. The lowest energy of the source should be less than or equal to ECUT. (Each card should have a pair of numbers, $E_i, S(E_i)$ = height of histogram in interval E_i to E_{i+1}.)

Item 26 - Time Specifications (Format I10)

NOT — Number of time values used to specify the time distribution. Items 26 and 27 should be omitted for a time-independent problem.

Item 27 - Time Distribution (Format 2E20.10)

Each of these cards should contain a time value and the corresponding integrated source up to that time, $\int_0^t S(t)dt$. The first entry should correspond to the longest time with the integral equal to 1.0. The first time entry should be greater or equal to the first entry of the output time bin boundaries. The last entry is for time equal 0 with the integral equal to 0.

Item 28 - Monodirectional Source (Format 3E14.5)

If ISO=1, the direction cosines of the monodirectional source with respect to the X,Y,Z coordinate axes should be entered. If ISO=0, omit this card. Do not use angular weighting in the source regions if a monodirectional source is specified.

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* See Appendix H.

Item 29 - Volume Computation Parameters (Format 3I10, 3E10.2)

NMA The number of rays to be fired for volume computation.

NST The number of rays in a statistical aggregate for the purpose of error computation.

IRSAVE The region number from which rays are to be fired.

X,Y,Z The X,Y,Z coordinates of the point from which rays are to be fired.

NOTE - if volumes are precomputed and no volume computation is needed, Item 29 is a blank card.

Item 30 - Precomputed Volumes (Format I10,E10.3)

IP Region number of precomputed volume.

VP Precomputed Volume.

NOTE - if no precomputed volumes are supplied Item 30 is a blank card. As many precomputed volumes as desired (in ascending region number) may be supplied. In any case, the last card must be blank. If no volume computation and no precomputed volumes are desired, then 2 blank cards corresponding to Items 29 and 30 are supplied. This effects the default option of 1.0 for all the volumes.

Item 31 - Fast Slowing Down Option

A blank card will cause this option to be ignored. Otherwise, for air over ground problems only:

(a) (Format 4E10.4)

ECTE Neutron energy (eV) below which option is invoked.

STMAX Lateral extent in cm. (from source center) of slowing down region (internally squared).

ZS Source height in cm.

RS Source radius in cm. (assumed spherical source region).

(b) (Format I5/(6E10.3))

NALT — Number of air layers of constant density plus one (ground layer).

[ZBD(K),DFR(K),K=1,NALT] — Pairs of values for lower layer boundary and corresponding layer density factor (ground and contiguous air layer factors set to 1.0 internally).

ZBD(NALT+1) — Upper layer boundary of uppermost air layer, defining upper boundary of slowing down region.

End of data.

5.4 Organization of the SAMCAR Program

The SAMCAR program comprises a small main program, a supervisory routine (the effective main routine), and associated subroutines. The main program (SAMCAR) establishes certain array dimensions and initializes several flags. The supervisory routine (AMCAR) controls the entire calculation, calling the input processing routines (GENI and INPUTD), and the principal Monte Carlo routine (CARLO). In addition, the supervisory routine controls the operation of superbins. A number of labeled common blocks are used, some of which are described in detail in subsequent sections of this report.

5.4.1 Description of Routines

This section gives a brief description of every routine in the program. The routines which have an asterisk (*) superscript are of major importance. Routines which follow the main program description are given in alphabetical order. The brief descriptions are followed by detailed descriptions of the important routines.

ROUTINE	DESCRIPTION
SAMCAR	The main program. It establishes the dimensions of the MASTER and MISTER arrays, initializes certain flags, and reads the first binary record of information from the processed perturbation data tape (created by SAMIN and modified by SAMSAM and SAMGAM for a secondary gamma problem). Control is then passed to the supervisory routine, AMCAR.
AMCAR*	The control routine for the Monte Carlo calculations. This routine reads the remainder of information from tapes written by the previous jobs SAMIN and SAMSAM or SAMGAM for a secondary gamma problem. It manipulates the organized data tape (ODT) and the supergroup tapes. This routine also writes on tape the scores for each statistical aggregate for later use by the edit program SAMOUT.
ANISOT	A routine to pick a CHI value which will give the cosine of scattering angle, θ, in the case of anisotropic scattering.
ARG*	The general angle reselection routine of the bounded estimation procedure.

ROUTINE	DESCRIPTION
ARPREP	A subordinate angle reselection routine called by ARG. This routine implements the special reselection procedure which is required for "hydrogen-type" neutron scattering, i.e., scattering in which the effective mass of the recoiling nucleus is ≤ 1.0. The relevant analysis is given in Appendix E.
ASSIGN	A routine to assign IP's (perturbations) of specific types of corresponding problems. It returns an array IPROB(I,J), where I=1, total number of problems; and J=1, 11. IPROB(I,11)=NIP, number of IP's affecting the Ith problem. IPROB(I,1 to NIP) gives all the IP's for the Ith problem.
CARLO*	The correlated Monte Carlo calculation routine. The routine performs tracking, and controls importance sampling, collision events (via calls to CARSCA), and track length scoring.
CARSCA*	This routine, called by CARLO, controls collision events.
DIREC	Using a direction vector $\bar{W}$ as a polar axis, a direction $\bar{W}'$ is generated, the cosine of whose polar angle is CSTHT and with random azimuthal angle. Thus, new direction cosines $\bar{W}'$ are computed such that $\bar{W}\cdot\bar{W}'=\text{CSTHT}$ The routine is used in computing the new direction after a scattering.

ROUTINE	DESCRIPTION
DR1*	This routine calculates the unperturbed and perturbed macroscopic total cross sections as a function of energy for a given composition. It also computes the sampling distribution for picking the element of reaction.
DR3*	The collision mechanics routine. This routine picks the element of reaction and the reaction type. For Klein-Nishina scattering, it governs flux estimation at point detectors via calls to FLUP.
DR31*	This routine is called by DR3 when an elastic scattering event has been picked. It governs flux estimation at point detectors via calls to FLUP, determines energy and angle after scattering, and governs the weight adjustment of each problem (unperturbed and perturbed).
DR32*	This routine is called by DR3 when an inelastic event has been picked. It performs the same functions as DR31.
DR33	This routine computes the probability of scattering by a given angle in the lab system and the resulting energy. It calculates the common factor (lab/c.m. Jacobian) and calls DR35 or DR36 for the problem dependent c.m. factor, for elastic or discrete inelastic scattering, respectively*. It is utilized by FLUP in the BFAP estimation procedure, and by DR34 in the angle reselection procedure.

* Continuum inelastic is currently treated as isotropic in the c.m.

ROUTINE	DESCRIPTION
DR34	This routine, called by DR31 and DR32, initiates the angular reselection procedure by performing the preliminary position checking (see Appendix F) and then calling ARG and DR33 for reselection and weight adjustment.
DR35	This routine, called by DR33, SAMPIC and XWADJ, computes the weight adjustment factor for every problem (PAIPP array) given a value of CHI for an elastic scattering event.
DR36	This routine, called by DR33 and XWADJ, is the inelastic scattering counterpart of DR35.
FLUP*	This is the flux-at-a-point estimation routine. It is called by AMCAR for source particles and "FLUP" latents, and by DR3, DR31, and DR32 for Klein-Nishina, elastic, and inelastic collisions, respectively.
GARB	This is one of the routines of the Combinatorial Geometry Package (CGP). It is subordinate to the principal CGP input processor, GENI, and is utilized whenever the ARB body is specified on input.
GENI	The major geometry input processing routine. The routine reads geometry data, checks for errors, and puts the data into the MA and FPD arrays in the form required by the tracking routines.
GETIR	Another member of the CGP (as signaled by its leading character). This routine, called by INPUTD, determines the physical region of a point detector, given its position coordinates.

ROUTINE	DESCRIPTION
GG	The distance calculating routine of the CGP. Given a position X, a direction $\overline{W}$ and a body number, the routine computes the two distances RIN, ROUT measured from X to the body.
GP	An auxiliary routine called, as an option, by G1 for debugging printout.
G1	The main geometry tracking routine. Given a position X, a direction $\overline{W}$, and a region IR, the routine will calculate the distance 'S' from the point X to the next region in the direction $\overline{W}$. The routine also determines IR', the next region to be encountered.
INGRAL	An auxiliary routine called by SOUPIC to normalize histogram
INPUTD	The Monte Carlo input routine. The routine reads Monte Carlo input data and stores it in the MASTER array for use by the calculation routines. Region and point detector specification, importance sampling data, and output energy meshes are handled by this routine.
PACK*	A routine to store the position, direction, energy and weight data for a particle into 24 computer words. The 24-word records are used for latent storage and for output onto the interaction/transmission tape.
PICK*	The control routine for supergroup latents. This routine stores particles whose energies are not included in the supergroup currently being processed. These particles are stored by PICK in either the central memory or on tapes depending on the amount of core available for the particular problem.

ROUTINE	DESCRIPTION
RANF	The random number generator.
SAMPIC	A routine to pick a CHI value (which will give the angle of scattering at a given energy) from the sampling CHI-table. This routine (via DR35) adjusts the perturbation weight of each problem by multiplying into each problem weight the ratio of probability density of selecting this CHI-value from each particular distribution over the sampling distribution.
SAMPIE	A routine to pick an ENN-value (the emerging energy in the event of continuum inelastic scattering) from the sampling ENN-table. This routine also adjusts the perturbation weight of each problem by multiplying into each problem weight the ratio of probability density of selecting this ENN-value for each particular distribution over the sampling distribution.
SEEK*	Given a vector ET with elements monotonically decreasing or increasing, and a variable E, this routine will search through the ET and determine the bin containing E.
SOUCAL*	The input processor for the source information required by the Monte Carlo routines for primary neutron problems. The routine processes energy and time spectrum data, and source region data. The data are stored in the MASTER array.
SOUPIC*	A routine to generate initial source particles. The routine uses the source information processed by SOUCAL and delivers position, energy, time, direction, and weight data for source particles. It also reads in source data from an external source tape.

ROUTINE	DESCRIPTION
TALLY*	A summary routine. The routine prints a one line summar of results for each statistical aggregate. Quantities s as number of collisions, absorptions, degradations, birt and deaths are printed for each aggregate.
TERP	A linear interpolation routine.
TIME	This routine interrogates the machine clock routine. It is utilized by AMCAR, TALLY, and VCALC.
TRALA*	This routine is called by FLUP to compute the problem de pendent array of optical pathlengths between collision (source) point and a detector point.
TROPIC	A routine to generate a vector of direction cosines from isotropic distribution.
UNPACK*	A routine to unpack a 24-word vector containing position direction, energy, and weight information.
UNPR	A routine to retrieve from the MASTER array six integer variables and to deliver the six integer variables store in the common block labeled REGPAR.
VCALC	The volume computation routine. Region volumes are com- puted by numerical integration.
WRT14	A routine to write 24-word records onto tape. The routi is called whenever a transmission or interaction is to h put on tape.
XWADJ(IEL)	This routine (in conjunction with DR35 and DR36) adjusts perturbation weight of each problem in case a perturbati of angular distribution exists. IEL=1, for elastic scat ing; IEL=2, for inelastic discrete scattering. This rou tine is called only when there is perturbation but no sampling table is available. The selection of angle of scattering in this case is from the unperturbed distrib

Effective Main Program - Subroutine AMCAR

AMCAR controls the Monte Carlo subroutine (CARLO) and arranges storage allocation for supergroups. As noted in Section 4.2, BAND arranges cross sections in certain energy bands. The output energy bins are also arranged in certain output supergroups. Cross section input corresponding to a sing band can be stored in computer memory at a given time. Scores correspondin to a single output supergroup can be stored in computer memory at any given time. The two meshes (bands and output supergroups) do not necessarily co-incide. A combined mesh defines a set of superbins.

AMCAR starts by reading in the highest energy cross section band, and arranging the memory for the highest energy output supergroup. The highest of the low-energy bounds of these energy ranges defines EBL, the low energy the superbin currently treated.

The program then calls the source-picking routine SOUPIC, and examines the energy E. If $E \leq EBL$, the particle is stored as a latent by calling the storing part of subroutine PICK, and SOUPIC is called again. When $E > EBL$, s routine CARLO is called*. CARLO tracks the particle, scores contributions fluxes when needed, and distributes collisions along their track. Particle coming out of collision are also tracked if their energy is above EBL; part coming out of collision with $E \leq EBL$ are stored as latents by calling PICK. trol is finally returned to AMCAR, which proceeds to the next source partic This process is repeated until a complete statistical aggregate of particle has been treated for the highest energy superbin.

* If the run involves point detectors (i.e., NDET≠0), the call to CARLO is preceded by a call to FLUP.

At this point, AMCAR switches to the next energy range by either reading a new band of cross section data, or by writing out on tape the set of scores obtained and preparing the memory layout for the next supergroup, or both. It then proceeds to call the retrieval section of subroutine PICK, which picks latents from previous superbins. If E≤EBL, the particle is stored again as a latent by calling PICK. If E>EBL, CARLO is called*. The procedure continues until all latents have been examined, at which point AMCAR switches to the next superbin, etc., until the low-energy cutoff is encountered. When this occurs, AMCAR switches to the highest superbin, and proceeds to treat the next statistical aggregate of particles. The calculation terminates when a history number exceeds the cutoff value NHIST specified on input. A 'blank' interaction record, with NHIST=NHIST+1, is written on the interaction tape and all tapes are rewound.

Subroutine ARG

This is the general angle reselection routine of the bounded flux-at-a-point (BFAP) estimation procedure. Together with its auxiliary subroutine ARPREP, it implements the algorithms described in Appendices E and F. A non-mathematical description is given in this section.

Subroutine ARG is called by SOUPIC when a source direction has been picked, or by DR34, following the selection of a post-scattering direction. In either case, this initially selected direction will be reselected, if the selected ray intercepts the sphere of influence, or "critical sphere", around a "live" detector, i.e., a detector whose scoring capacity is currently active. This angular reselection procedure comprises three distinct stages: (1) direction checking; (2) reselection of angle; (3) weight adjustment.

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* If a "FLUP" latent is PICK-ed (J12345=5), FLUP is called instead of CARLO.

In the direction checking stage, the orientation of live detectors with respect to the originally selected ray is analyzed. If the ray does not intersect any detectors, reselection is bypassed. If an intersection is found, reselection may be necessary, but prior to reselection, potential "conflicts" must be resolved. Two types of conflicts are possible: (1) the intersected critical sphere overlaps the critical sphere of another live detector; (2) the cone, with vertex at the collision (or source) point, which is tangent to the intersected critical sphere, overlaps the corresponding cone of another live detector. A conflict is resolved by Russian roulette, in which all detectors, but one, are deactivated.

Subsequent to the direction checking stage, at most one live detector sphere is intersected by the originally selected ray. If such an intersection has survived, a new direction is selected in the reselection stage, as described in Appendix E.

The final stage in the reselection procedure involves the calculation of a weight adjustment factor which compensates for the biasing introduced by reselection.

Subroutine CARLO

This is the Monte Carlo calculation routine. It controls importance sampling, collision mechanics, and scoring.

Each source particle is accompanied by its associated array of problem weights, F_i, i=1,2,...,NPROB, where NPROB is the number of problems.

Source particles generated by subroutine SOUPIC, as well as latents, are tested on energy. If the energy is below the lower bound of the current superbin it is stored as a latent. Otherwise it is transmitted to CARLO, which tracks, distributes further collisions, if any, and scores answers.

When point detectors are being used, and if the extended particle path passes sufficiently close to a specified detector, preliminary geometrical calculations necessary to bias the collision positions are carried out. This biasing is required to make flux estimates for point detectors bounded.

Given the region number IR, the energy E, source particle position vector XB, and the direction of flight WB, a sampling weight $W=W_{IR}.W_{E}.W_{WB}$ is calculated.

The subroutine DRl is called, which provides the total macroscopic cross sections μ_i, i=1,...,NPROB, for each of the problems.

The geometry routine $Gl(S_1)$ is called to provide the distance S_1 to the first region boundary encountered from XB in the direction WB. Gl also produces IR', the region number on the other side of the boundary, and X', the point of intersection of the track with the boundary. If IR is a scoring region, the contribution $\emptyset_i$ to the flux is calculated and stored for all problems, where

$$\emptyset_i = (F_i - F_i e^{-\mu_i S_1})\frac{W}{\mu_i}, \quad i=1,\ldots,NPROB.$$

Once the tracking and scoring (if called for) are completed, the Monte Carlo procedure necessary to generate collision positions is invoked. This procedure uses three different algorithms, depending on whether or not the special biasing for bounded estimation of point detectors is needed, where the special biasing can use either of two algorithms.

The general principle used for the selection of collision positions involves an implicit splitting and Russian roulette procedure. Specifically, to select the positions, an unnormalized probability density f(s) is defined, where s is distance along the track, and the expected total number of collisions is given by $I=\int_0^\infty f(s)ds$. The actual number of collisions is then either [I] or [I]+1, where the probability of the additional collisions is I-[I], where [x] = the greatest integer less than or equal to x.

In carrying out the collision dropping procedure, f(s) is treated in a piecewise fashion, where in each interval f(s) and its indefinite integral have the desired analytical properties, most important being that the indefinite integral be easily invertible. Finally, to compensate for any biasing involved in using f(s), the particle weights $\{F_i\}$ must be adjusted accordingly.

The remainder of the procedure involves the definition of f(s), which may assume three forms, as a consequence of bounded biasing. The algorithms which have been implemented are described in Appendix E.

If a collision is dropped by means of the above-described procedure, subroutine CARSCA is called to complete the remainder of the processing. When all the collision positions have been selected, the subroutine proceeds, as follows.

A test is made to determine whether the next region is a transmission region* (if it is, the coordinates S', IR', energy, time, etc., are written on tape), and whether it is the escape region. If it is not the escape region, the particle is moved to the boundary by setting IR=IR', by computing the new region weight W_2, and by setting $F_i=(\frac{W_1}{W_2})$, where W_1 is the old region weight.

We again define FMAX = the largest of F_i's and play another game of chance. If FMAX$\leq F_z$, the particle is either killed, or it survives with the F_i's renormalized by dividing all of them by FMAX. If FMAX$\geq F_z$, DR1 is called to provide the new total macroscopic cross sections for all problems and control is transferred to the section which calls the geometry routine G1(S_1). The tracking continues until a kill occurs or the escape region is reached.

---

*Not used with point detectors.

After the tracking is completed, the latent table of particles within the current energy superbin is examined. If the table is not empty, the last latent is picked up and processing continues. (Latents are created in CARSCA). The subroutine is terminated when the latent table is exhausted.

Subroutine CARSCA

This routine controls all the processing necessary after a collision position is selected in CARLO. The particle weights are adjusted to compensate for the biasing used in the sampling. Subroutine DR3 is called to carry out the scattering mechanics, producing new energy and direction.

If the scattering event was absorption, or if the energy was below the cutoff, the procedure is terminated. If not, a sampling weight is calculated and Russian roulette is played if the comparison with FZ warrants it. Finally, if not terminated, the particle is stored as a latent in one of two lists, depending on whether or not the energy is within the energy superbin being considered. Moreover, if it falls within the current superbin, a Russian roulette procedure may be necessary, if the list is full, in order to make space available. The procedure terminates after completion of latent storing.

If an interaction tape is being created, for subsequent use as a source of secondary radiation, CARSCA will oversee the proper storing of the parameters of the interaction event. This includes both absorption and scattering events.

Subroutine DR1

This routine computes the unperturbed and perturbed macroscopic total cross sections at a given energy for a given composition. It first picks up all the relevant perturbations (IP's of type 1, 2 and 3 of relevant elements). Then DR1 calls subroutine ASSIGN to assign the perturbations to each problem and proceeds to compute the macroscopic total cross section for each problem

according to the perturbation description of each problem. When called by CARLO, DR1 also computes the sampling probability distribution for picking the element of reaction. The latter computations are bypassed when DR1 is called from FLUP or TRALA during BFAP estimation, as signaled by the integer flag, IFA=1.

Subroutine DR3

Subroutine DR3 is called by CARSCA to perform the actual collision mechanics. It returns to CARLO with a new energy (EPRIM), a new direction (WP), the cosine of the scattering angle (CSTHT), and an integer (NCDB) denoting the type of interaction event. The types of interaction are listed below:

NCDB	Interaction
1	discrete isotropic inelastic scattering
2	discrete anisotropic inelastic scattering
3	isotropic elastic scattering
4	anisotropic elastic scattering
5	Klein-Nishina gamma-ray scattering
6	absorption
7	continuum isotropic inelastic scattering
8	continuum anisotropic inelastic scattering

DR3 first picks the element of reaction from the sampling distribution computed in DR1, and adjusts the perturbation weight for each problem. It then computes the sampling distribution for the selection of a reaction type for the chosen element.

Subsequent to the selection of a reaction type, control is passed to either DR31 (for elastic scattering) or DR32 (for inelastic scattering) for the selection of post-scattering direction and energy.

Subroutine DR31

This routine is called by DR3 subsequent to the selection of an elastic scattering event. Its basic function is to compute a post-scattering direction and energy. In addition, if point detectors have been specified on input, the BFAP estimation procedure is initiated by calling FLUP.

When a perturbation of angular distribution exists (type 2 or 6) at the collision energy E, DR31 will call SAMPIC to pick a value of CHI from the sampling CHI-table (if it exists). SAMPIC adjusts the problem-dependent perturbation weights automatically. If a sampling table is not available, DR31 will pick a CHI from the unperturbed distribution, and call XWADJ to adjust the perturbation weights.

Finally, if point detectors have been specified, the angular reselection procedure is initiated with a call to DR34.

Subroutine DR32

This routine is called by DR3 if an inelastic scattering event has been selected. Its basic functions are the same as those of DR31 for elastic scattering, including FLUP and DR34 calls for BFAP estimation and angle reselection, in the event that point detectors have been specified.

When a perturbation of secondary energy distribution exists (type 2 or 7) at the collision energy E, DR32 will call SAMPIE to pick a value of ENN from the sampling ENN-table (if it exists). SAMPIE adjusts the problem-dependent perturbation weights automatically. If a sampling table is not available, selection is made on the basis of the unperturbed data, and perturbation weight adjustment is performed within this routine.

Subroutine FLUP

This routine performs the BFAP estimation for each live detector. It is called by AMCAR for each source particle (the primary source must be isotropic) and for "FLUP latents" (i.e., pseudo particles, established in a previous call to FLUP for estimation tracking, whose energy fell below the then current superbin cutoff). It is also called by DR3, DR31, and DR32 for Klein-Nishina, elastic, and inelastic collisions, respectively.

The estimator scored is an array, each element of which is given by

$$W_i g_i(\cos\theta)\, e^{-S_i}/4\pi r^2, \quad i=1,\ldots, n$$

where n = the number of problems;

W = net particle weight, adjusted for all sampling biasing that may have taken place previously;

$g_i(\cos\theta)$ = probability of scattering through an angle of cosine θ, (or 1 for an isotropic source);

S = optical distance between collision (or source) point and detector point;

r = problem independent, geometric equivalent of S.

At a collision point, the g_i-array is computed by calling DR33, which also returns an energy EP, the lab energy resulting from a pseudo-scattering in the direction of the detector. If EP is below the current superbin cutoff, all the information already computed for the estimator ray is stored (via calls to PACK and PICK), to be picked-up later as a "FLUP latent". The S_i-array is computed via subroutine TRALA.

The detectors, for which a flux estimator is computed, are determined as follows: For a "FLUP latent", only the detector which was being treated at the time of the latent store is treated. Otherwise, the variable KDLIV (see Appendix F) is examined. For KDLIV$\geq$0, all detectors are "alive", i.e., their

scoring capacity is active. But for KDLIV<0, only detector # -KDLIV is "alive", as a result of Russian roulette, which was performed to resolve a reselection "conflict" (see Appendix F and the discussion of Subroutine ARG). In the latter case, only detector # -KDLIV is treated, with an additional weight adjustment factor NDET (the total number of detectors), which compensates for the Russian roulette biasing.

Subroutine PACK (X,WX,E,IR,T,IDET,W,NHIST,WC,J12345,F,P)

This subroutine transfers the items in the calling sequence to the P array. The relationship between the arguments and the array P is shown below:

Argument	P	Definition
X(1)	P(1)	
X(2)	P(2)	Position Coordinates
X(3)	P(3)	
WX(1)	P(4)	
WX(2)	P(5)	Direction Cosines
WX(3)	P(6)	
E	P(7)	Energy
IR	P(8)	Region Number
T	P(9)	Time
IDET	P(10)	Detector Number
W	P(11)	Sampling Weight = $(W_{IR} \cdot W_E \cdot W_{WB})$
NHIST	P(12)	History Number
WC	P(13)	Weight (carry-along weight, usually =1.)
J12345	P(14)	Particle Type (defined below in description in PICK routine)
F_i	P(14+i)	Problem-dependent weights, i=1,...,10

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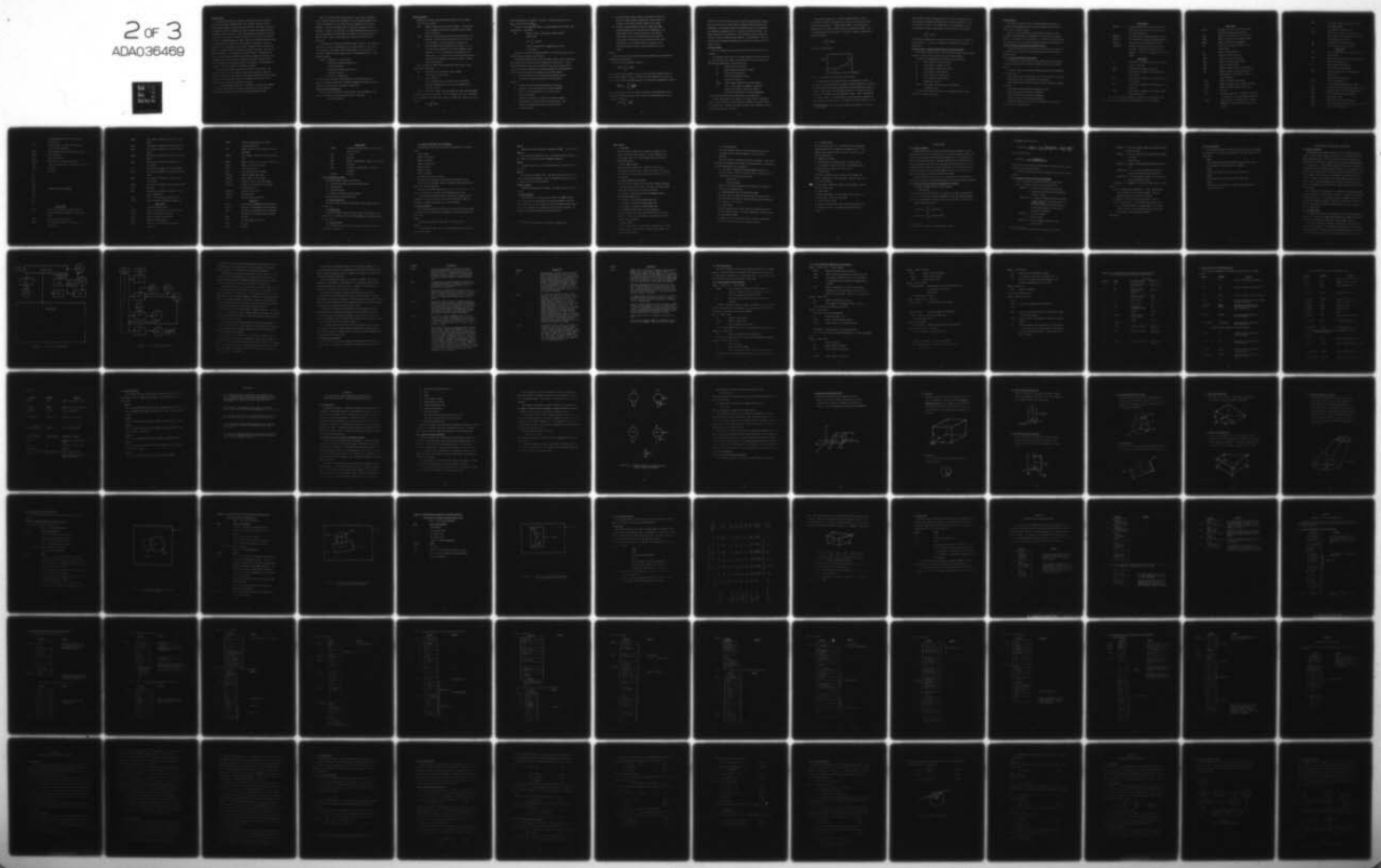

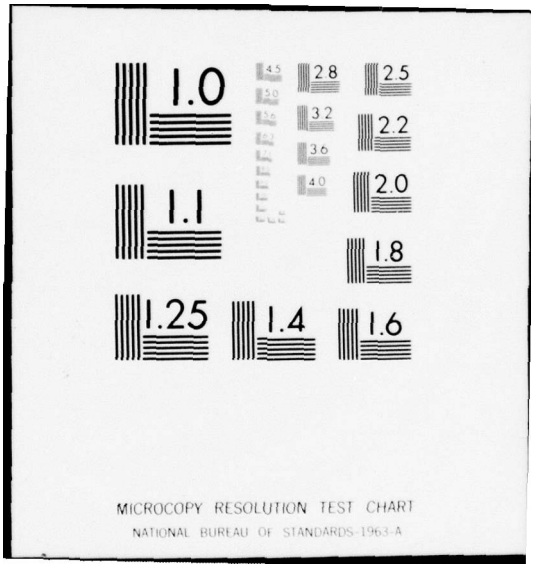
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Subroutine PICK

We have seen throughout the previous sections that particles degraded below the energy EBL, low-energy limit of the superbin currently treated, were stored as latents by calling the subroutine PICK. They were later picked up by AMCAR by calling the subroutine PICK. The subroutine INPUTD allocates the memory to data, scores, etc. The remaining memory is assigned to the subroutine PICK, to be used as a buffer for latents. One 'end' of the buffer is assigned to 'degraded' particles. This is the end of the buffer where particles are being stored. The other 'end' of the buffer is assigned to 'unsorted' particles, i.e., the particles to be picked. Associated with each end of the buffer is a magnetic tape to be used when the buffer overflows. There are two modes of operation. In one mode, the top of the buffer is unsorted and the bottom is sorted. When the switch is made from one superbin to the next, the 'unsorted' part is empty, and the 'degraded' part may have particles which become 'unsorted' for the supergroup about to be treated. The designation of the buffers (and of the tapes) is, therefore, switched.

There is no set boundary between the two 'ends' of the buffers. The number of particles in the 'unsorted' buffer keeps decreasing, whereas the number of particles in the 'degraded' buffer keeps increasing, and can increase faster than the other number decreases. Therefore, the two parts of the buffer can meet, causing an overflow of the buffer.

It is then determined which 'end' of the buffer is longest, and a number of particles exactly equal to one-half the total length of the buffer are written from the longest 'end' onto the corresponding magnetic tape.

When the 'unsorted' buffer becomes empty, a test is made to determine if any 'unsorted' particles are available on the corresponding magnetic tape. If none are available, the calculation has been completed for the current superbin. If some are available, they are read into the buffer if room is available. If room is not available, it is made available by writing out part of the other buffer on the other tape; the length of the record written out from one 'end' is equal to the length of the record to be read into the other 'end'.

The subroutine PICK deals with different kinds of latents. The quantities stored are: X,Ω,E,IR,T,I,W,NHIST,WC,F_i's and J12345, where X is the position, Ω the direction, E the energy, IR the region number, T the time, W and F_i's the weights, NHIST the history number, and WC a normalization factor. I and J12345 are indices.

J12345 = 1 identifies a source particle

= 2 identifies a particle coming out of elastic scattering.

= 3 identifies a particle coming out of inelastic scattering.

= 5 identifies a FLUP latent

(In other parts of the code, J12345=6 identifies a transmitted particle, J12345=7 an inelastic interaction, J12345=8 an absorption, J12345=9 an elastic interaction, and J12345=10 a non-elastic interaction.)

Subroutine SEEK (E,EOUT,NOUT,I)

Given the vector array EOUT, of length NOUT+1, and the argument 'E' the routine will perform a binary search and return 'I' such that

$$EOUT(I) \leq E < EOUT(I+1).$$

Subroutine SOUCAL

SOUCAL will read source data and prepare tables for use by SOUPIC.

The first card contains:

NSR — Number of regions where the source extends. If this number is 0, an external source tape is expected, and no further input is required.

IFLAG — Number of energies used to define the source spectrum. The spectrum is specified later in input which is in the form of a histogram. It will be defined by IFLAG entries.

ISW — Switch determining the normalization of problem. If it is 0, fluxes will be normalized to a single (unbiased) source particle. If it is 1, fluxes will be normalized to the 'total power', i.e., output will be flux per source particle, multiplied by the summation (over source regions) of power density times volume.

This is followed by (NSR) cards specifying the (NSR) source regions. Each of these cards gives:

ISR — Specification of a geometrical region number.

P — Power density in that region.

ISO — ISO=0, isotropic,

ISO=1, monodirectional. If ISO=1 in any of the (NSR) regions, a monodirectional source will be assumed in all the (NSR) regions.

After this follow the (IFLAG) cards specifying the energy spectrum assumed to apply to all the source regions. This is a table of E vs. S(E) = the height of the histogram to the right of the energy E. SOUCAL will compute the integral spectrum

$$F(E) = \int_E^{\infty} S(E)dE.$$

Linear interpolation is assumed on E vs. F(E). The first entry must be for $E \leq E_{cut}$, and the last for $E \geq E_{high}$.

If there is time dependence (NT>0), the time dependence of the source must be specified. A card gives:

NOT — Number of cards. This card is followed by NOT cards giving

$$t \text{ vs. } \int_0^t S_t(t)dt.$$

Linear interpolation is assumed between entries in the table.

Finally, if the source is monodirectional, the projections $\Omega_x, \Omega_y, \Omega_z$ of the direction must be given on the last card.

The subroutine SOUCAL reads in all this input, prints it back, and pre-computes tables to pick directly from the biased source distribution. Since we allow perturbations of the source spectrum which are input as density functions in the form of histograms, two preliminary steps are necessary before we have the final biased source distribution for subroutine SOUPIC:

1. Form the envelope of the unperturbed and perturbed spectra,
2. Calculate the distribution function of this envelope.

Step (1)

a. Normalize each source spectrum between E_{cut} and E_{high}.
b. Construct a table containing all the energy boundaries present in the specifications of the various source spectra (histograms).
c. Rearrange this table into a monotonic increasing sequence.
d. Remove duplicate energies from the ordered sequence. This provides a combined energy table for calculating the envelope spectrum.

e. For each energy E surviving step d, call SEEK to locate it in each of the input spectrum energy-tables, and calculate the strength of each source spectrum (dp/dE) at this energy.

f. For each of these energies E, take the maximum individual spectrum strength as the envelope value corresponding to the energy range from E to the next higher E in the combined energy table. Since the individual spectra are assumed to have piecewise constant dp/dE, and the combined energy table includes all of the histogram energies, no details of any spectrum-structure are lost in this construction of the envelope.

Step (2)

Calculate the envelope integral spectrum and normalize it, and we have the sampling source spectrum S(E).

The code first pre-computes a table of

$$\text{SPEC}(I) = \int_{E_I}^{\infty} S(E)dE,$$

where the E_I's take the values of E_{high}, of all the energy boundaries where the energy weight changes, and E_{cut}. The code then runs through all the source regions and, for each new energy-importance set encountered, pre-computes a table of

$$\widetilde{\text{SPEC}}(I,J) = \int_{E_I}^{\infty} \frac{S(E)dE}{W_E(E)}$$

where J runs from 1 to the total number of different energy-importance sets encountered in the source regions; also for each new angular importance set encountered, a table

$$P(I,K) = \int_{\omega_i}^{1} \frac{d\omega}{W_\omega(\omega)}$$

where the ω_i's take the values of cosθ at which the angular weight changes, and K runs from 1 to the total number of different angular importance sets encountered. The different tables are renormalized and both the modified and unmodified integrated source are computed in each source region. The former quantities are proportional to the probability with which particles should be picked in different source regions. A table SOUR(L) is built up, which gives the cumulative probability for a source to be picked in the M^{th} region for $M \leq L$.

Subroutine SOUPIC

This is a subroutine which picks particles from the biased source distribution.

If an external source tape is to be used, groups of 35 source particles are read from tape into a buffer, and returned one by one to the main code. The quantities describing a source particle are:

XB	Coordinates of the particle
IR	Region number where particle is born
WB	Direction of the particle
T	Time at which particle is born
E	Energy of the particle
NHIST	History number attached to the source particle
F_i	i=1,..., total number of problems. Statistical weight of the particle (usually set equal to unity if no perturbation of the source spectrum).

The procedure for internal source generation is outlined below.

A first random number ξ is compared to the table SOUR(L) (computed by SOUCAL). The smallest L for which SOUR(L)$\geq$ξ determines the region IR=ISR(L) to be picked from. Standard techniques are used to pick coordinates of points uniformly distributed in a region.

The energy is picked next. A stratified random number (called CE in the code) is obtained (stratification is done for each statistical aggregate of source particles). A biased random number $\bar{\xi}$ is then obtained by interpolation in the SPEC vs. SPEC(J) tables pre-computed by SOUCAL. (The J is determined by the region number.) Finally, the energy is determined by solving the equation

$$\bar{\xi} = \int_{E}^{\infty} S(E)dE$$

using linear interpolation.

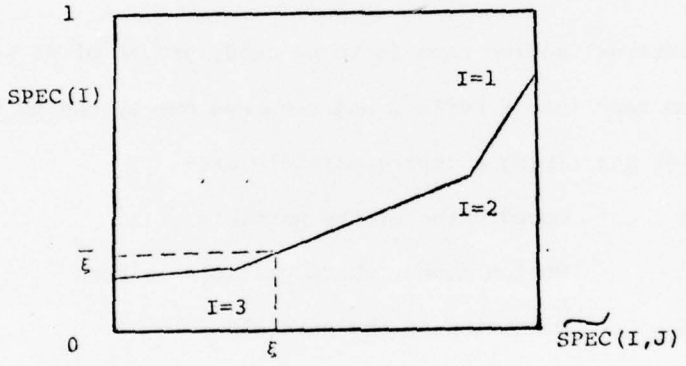

Figure 2 - Selection of $\bar{\xi}$ for Picking a Source Energy

The direction WB of the source particle is determined as follows. If the source is isotropic and there is angular importance sampling, the cosine of the angle between the particular aiming angle and the direction is chosen by picking a random number, and interpolating between the angular mesh supplied on input vs. the table P(I,K) pre-computed by SOUCAL. (The K is determined by the region number.) A random azimuth is then picked, which completes the specification of the direction*. In the absence of angular importance in the

* If point detectors exist, the angular reselection procedure is initiated by calling ARG.

source region, standard techniques are used. The case of a monodirectional source also can be handled, provided there is no angular importance in the source region. Finally, if time dependence is to be determined, a time T is determined by another random number ξ and the solution of the equation

$$\xi = \int_0^t S_t(t)dt.$$

The quantities communicated to the main code are XB, IR, WB, T, E, NHIST, W, and W_c where (W_c = 1), and W is the weight in the region IR at energy E in the direction WB.

Subroutine TALLY (J,NHIST,NCOL,NDEG,NABS,FKILL,BIRTH,ESCAP,NRMAX)

The routine is used to print a tally at the end of each statistical aggregate and to print a tally by region at the end of the problem.

At the end of each aggregate the following items are printed.

NC	Total number of collisions thus far
ND	Total number of degrades thus far
NA	Total number of absorptions thus far
FK	Total number of kills thus far
BI	Total number of births thus far
ES	Total number of escapes thus far
T	Elapsed time thus far
JCOUNT	Total number of particles on the interaction/ transmission tape.

The same items, except for ES and T, are printed at the end of the problem as a function of region.

Subroutine TRALA

This routine is called by FLUP, in the BFAP estimation procedure, to compute the problem-dependent array of optical distances from collision (or source) point to a detector point.

Given an intial point $\overline{XB}$ and a direction $\overline{WB}$, the routine will track from $\overline{XB}$ in the direction $\overline{WB}$. The tracking will continue until the geometric distance to the detector has been reached, or, as a result of Russian roulette, the estimator is set to zero to reduce unproductive tracking (see Appendix G).

Subroutine UNPACK (X,W,E,IR,T,IDET,F,NHIST,WC,J12345,P)

Subroutine UNPACK distributes the 24-word P array among the variables in the argument list according to the correspondence shown in the discussion of subroutine PACK.

5.4.2 Glossary of Important Variable Names

The following is a brief outline of major common blocks in the program. A detailed description of each variable in common is given on the following pages.

The "blank" common block contains the master storage array and frequently used input arrays.

Common REGPAR contains six parameters used in the Monte Carlo calculations.

Common INPUT contains non-subscripted input parameters.

Common PAREM contains position, direction, energy and importance sampling parameters.

Common COMPUT contains parameters computed from input.

Common CROSA contains cross section parameters.

Common FAP contains flux-at-a-point parameters.

Common SOU contains source-dependent parameters.

Common PUTAD contains data controlling the parameters to be written on the interaction, transmission tape.

"Blank Common"

EOUT(100)	An array containing the output energy bins for flux results. The array contains all bins for all output supergroups.
EWTAB(50)	The energy mesh for energy importance sampling.
ANGLE(50)	The cosine mesh for angular importance sampling.
TTAB(50)	The time mesh for time-dependent problems.
ASTER(5000)	The master storage array containing input and flux data. A complete description appears in Appendix C. The array is equivalenced with array MASTER.

COMMON REGPAR

ISC	The location, in MASTER, of the flux scores for scoring region ISC.
NREG	The composition number for region IR.
IRW	The location, in MASTER, of the region weight for region IR.
IEW	The location, in MASTER, of the energy weight table for region IR.
IAM	The location, in MASTER, of the aiming angle for region IR.
IANG	The location, in MASTER, of the angular weight table for region IR.

Note that the above six items are all keyed to a region number, "IR". The six items are retrieved from the MASTER array by a call to UNPR.

Common INPUT

NSTART	The number of real time seconds of running time before terminating and editing.
NSTOP	Number of the last history to be treated.
NSTAT	Number of histories per statistical group.
NRMAX	Number of regions in the geometry.
NG	Either 0 for a neutron problem or 1 for a gamma problem.
NT	Number of output time bins.
NOUT	Number of output energy bins.
NUMSC	Number of flux scoring regions.
NRWL	Number of distinct region weights.
IREX	The escape region number.
NEWL	Number of energy bins for energy weighting.
NEW	Number of distinct energy weight sets. If NEWL and NEW = 0, the problem contains no energy weighting.
NAIML	Number of distinct aiming angles.
NUMANL	Number of angular bins for angular weighting.
NUMANG	Number of distinct angular weight sets.
JRT	Not used.
ECUT	Low energy cutoff (ev). Tracking of a particle is terminated if its energy degrades below ECUT.
ETHERM	Thermal energy if a thermal group is required. ETHERM must be within the energy limits of the problem.

TCUT	Time cutoff (equal to first entry of time bin boundary table).
FZ	See discussion in Section 5.4.1.
EHIGH	High energy cutoff (ev). This should be less than or equal to the highest energy for which cross sections are available.
EBL	Lower bound of the current superbin.
EBH	Upper bound of the current superbin.

Common PAREM

XB(3)	The X,Y,Z coordinates of the current particle's starting point.
WB(3)	The direction cosines of the current particle.
E	Energy of the particle.
IR	Region number of the particle.
T	Time of flight of the particle.
IDET	A detector number used in flux-at-a-point calculations.
F	Importance sampling parameter.
NHIST	Current history number.
WC	A weight parameter calculated by SOUPIC .
J12345	A particle type flag (see the discussion of PICK).
WP(3)	Direction cosines of particle after scatter.
XP(3)	X,Y,Z coordinates of current position.
EPRIM	Energy after scatter.
ATWT	Atomic weight of scattering element.
NCDB	Interation type indicator (see discussion of DR3).
CSTHT	Cosine of scattering angle.

U	Total macroscopic cross section at energy E for region IR.
LCHI	Location in the XS array of a table used in anisotropic scattering.
IATWT	Identification digit of the scattering element.
IERR	Error indicator.
IDBG	Debug printout flag.
IRPRIM	Next region to be entered by the ray.
NASC	A flag to initiate the G1 routine for a new ray.
LSURF	Not used.
XXX	Not used.
LRI	
LRO	
RIN	
ROUT	
KLOOP	
LOOP	Geometry subroutine parameters
LTYPE	
PINF	
NOA	
DIST	

Common COMPUT

NUMNOU	The product of NUMSC (the number of scoring regions) and NOUT (the number of output energy bins).
JONUM	An index used in flux scoring.
LNCNOL	The location in MASTER of the collision by region table.

LBIRTH	The location in MASTER of the birth by region table.
LREGT	The location in MASTER of the region data table.
LFKILL	The location in MASTER of the kills by region table.
LESCAP	The location in MASTER of the escapes by region table.
LLAST	The location of last word in MASTER used by the program.
NDQ	The size of the MASTER array (set in SAMCAR).
LNDEG	The location in MASTER of the degrade by region table.
LNABS	The location in MASTER of the absorption by region table.
LSCORE	The location in MASTER of the flux scoring array.
LPACK	Not used.
NTOT	NUMSC times (the number of energy bins in the largest supergroup).
LGEOM	The location in MASTER of geometry data.
LEGEOM	The last location in MASTER of geometry data.

Common CROSA

NB	Cross section band counter.
JUPPER	Indices in the ETOT array giving the energy
JLOWER	range of the current supergroup.
KPHYS	Number of physical compositions.
NELEM	Number of unique elements.
LENCHI	Length of the CHI-table for anisotropic scattering.

LENENN	Length of the ENN-table for inelastic continuum scattering.
NLOC	Number of words in the XS array for current supergroup.
NENERG	Total number of energies in the cross-section mesh.
NENBAN	Number of energies in the current supergroup.
NBAND	Number of cross section bands.
LENXS	Size of the XS array.
EBLX	Lower energy bound of the bands.
NAME(30)	Array of element identifiers.
ATTAB(30)	Atomic weight for each element.
LOCS(30)	Location in XS of σ_t for each element.
LOCLEV(30)	Location of the ELEV-table for inelastic discrete scattering.
LENPLV(30)	Length of the PLEV-table.
ETOT(500)	The energy mesh.
XS(5000)	The cross section data array.

Common FAP

XAD(25)	The array of X-coordinates for the detectors.
YAD(25)	The array of Y-coordinates for the detectors.
ZAD(25)	The array of Z-coordinates for the detectors.
ID	The number of the detector being processed.
NDFAP	Not used.
NDET	The total number of detectors.
LSCFAP	Not used.
LPAFAP	Not used.

Common PUTAD

IRT(10)	Transmission region numbers. Only the first three are used.
IWA	Not used.
IWI	Not used.
IWE	Elastic recording flag. Nonzero for recording.
IWD	Not used.
IWO	Non-elastic recording flag. Nonzero for recording.
OTHER(5)	Not used.

5.4.3 Description of Output

The printed output consists of four parts:

1. Title card and cross section band energy limits,
2. Geometry data,
3. Monte Carlo data,
4. Results of the Monte Carlo calculation.

These four parts are discussed below.

1. Cross Section Data

The printed lines are basically a repeat of input items 3 and 5 (see section 5.3).

2. Geometry Data

The printed geometry output is simply a repeat of input item 7 (see section 5.3). In addition, the storage requirements in the geometry arrays are also given.

3. Monte Carlo Data

As in Geometry Data, the Monte Carlo data are a repeat of the input data (items 8 through 30).

4. Results of the Monte Carlo Calculation

The program will print for each statistical aggregate the following items:

History number

Number of collisions

Number of degrades

Number of Absorptions

Number of kills

Number of births

Number of escapes

The elapsed real time in seconds.

The number of transmissions and interactions recorded on tape.

Note that all of the above items are cumulative and are printed as a single line for each aggregate.

When all the histories have been processed, a printout giving the total number of absorptions, inelastics, and transmissions will occur.

The previously discussed tallies as a function of aggregate will be repeated as a function of region. Thus, for each region the number of collisions, degrades, absorptions, etc., will be printed.

5.5 Tape Utilization

The following describes the function of each tape used in the program. Tape numbers refer to FORTRAN logical numbers. All tapes are used in the binary mode.

Tape 8

The processed perturbation data tape. (See Section 4.4).

Tape 10

The organized data tape (ODT). The tape contains cross section data for a given problem.

Tape 12

Sampling CHI- and/or ENN-tables, generated by SAMSAM. (See Section 4.4).

Tape 14

The interaction/transmission tape. All interactions and transmissions are written on this tape for use in subsequent problems.

Tape 15

An external source tape. The tape may also be the transmission part of tape 14.

Tape 16

The statistical aggregate tape. The AMCAR routine uses this tape to record each completed aggregate. The edit routines then process the tape to obtain the final flux, dose results.

Tape 17 & Tape 18

Temporary storage tapes for latents. The tapes are used by the PICK routine.

5.6 Error Messages*

Three types of error indications are given by the SAMCEP program. Type 1 errors give an error message and cause the program to terminate. Type 2 errors give an error message, but do not terminate the calculation. Type 3 errors terminate the calculation, but give no error message. The possible error stops and messages are discussed below.

---

* A discussion of BAND messages is included for completeness.

Type 1 Errors

1. SEEK ERROR

The error occurs in SEEK and is caused by an argument out of range of the vector being searched. The most probable causes are an input error in the output energy bins or the energy or angular weight bins.

2. OUT OF RANGE ON EBAND

The error occurs in BAND and is caused by the input cross section energy band mesh being outside the range of the energies on the EDT. The most probable causes are an input error or using the wrong EDT.

3. NO MORE ELEMENTS ERROR IN BAND

The error occurs in BAND and is given when an isotope identifier in the BAND input cannot be found on the EDT. The most probable causes are an input error or using the wrong EDT.

4. *** ERROR - BOTH FIRST AND LAST BIN BOUNDARIES MUST BE FLAGGED WITH NEGATIVE SIGNS

5. *** ERROR - EHIGH MUST BE WITHIN ENERGY BINS

6. **** ERROR - ECUT MUST BE WITHIN ENERGY BINS

7. **** ERROR - ETHRM MUST BE WITHIN ENERGY BINS

8. THE NUMBER OF ENERGY BINS IS TOO BIG THE MAX IS

The error indicates too many energy output bins to fit in the machine. The input must be modified. A suggestion is to allow another output supergroup.

9. ERROR IN NUMSC

The error occurs when a scoring region, as supplied by the region parameter input, is bigger than the input value of NUMSC. The input should be checked.

10. NO ROOM FOR DATA

The error indicates that the total room occupied by the input is greater than the allowable maximum. The input must be modified.

Note that errors (4) through (10) all occur in INPUTD. These errors will allow the remainder of the input to be processed but the program will not perform the Monte Carlo calculation.

11. **** ERROR - SPECTRUM NOT DEFINED BETWEEN EHIGH AND ECUT

The error occurs in SOUCAL and indicates that the energy spectrum violated one of the following constraints:

$$ECUT \geq ET(1)$$

$$EHIGH \leq ET(IFLAG)$$

where ET is the input energy spectrum and IFLAG is the number of entries in the spectrum table.

12. CANNOT HAVE ANG. IMP. FOR ANISOTROPIC SOURCE

The error occurs in SOUCAL and indicates that the special source direction option was used in a region containing angular importance. This condition is not allowed.

13. ERROR IN NOUT

The error indicates that a source energy was calculated by SOUPIC and is outside the range of the output energy mesh. Check the input.

14., BAD IRPRIM IN CARLO

An IRPRIM of zero was calculated in the G1 routine. The geometry input and the source position data should be checked.

15. S1 OUTSIDE BOUNDS

The error indicates that S1, the distance to the next boundary, as calculated by G1, is either zero or greater than 10^{11}. The geometry input should be checked. A more serious cause is an error in compilation.

16. ERROR IN SP IN CARLO

"S" the distance to the next collision is greater than S1, the total distance through the region. The FORTRAN statements in CARLO should be checked for a compile error.

17. ERROR IN NREG

A composition number of zero or greater than the KPHYS, the number of compositions, was encountered. Check the region input.

18. ERROR IN IRPRIM

A region number, IRPRIM, was greater than the number of regions. Check the region input.

19. ERROR IN ISC

A scoring region number, ISC, was greater than the number of scoring regions. Check the region input.

20. ERROR IN NCDB IN CARLO

An illegal interaction digit, NCDB, has been generated by DR3, the interaction routine. The cross section data should be checked.

6. PROGRAM SAMOUT

6.1 General Discussion

Program SAMOUT reads the scores for each statistical aggregate in supergroups from the output tape (IAGG=tape 16) of the previous program, SAMCAR, and writes a final cumulative statistical tape (NAGG=tape 4 in this program) from which all editing will be done. Subroutine EDIT will print the normalized flux with the percentage error for all the problems, and the differences (with their percentage errors) between all or any two problems. Once the cumulative statistical tape (NAGG) is written, program SAMOUT can be rerun using only the NAGG tape to edit any other problems or differences desired.

Response functions (cf. Section 5.2.7) will be read in at the time the IAGG tape is processed; the response functions of 1.0 are built into the program.

6.2 Description of the Flux and Percentage Error Calculation

The output of SAMCAR consists of flux integrals

$$F(IR,IE,IT,IA)$$

integrated over scoring region IR*, over energy bin IE, time IT, and given for all IR, IE, IT, for each statistical aggregate IA, IA=1, NOA, where NOA=NHIST/NSTAT. The normalization is NSTAT times the one specified by the SOUCAL input.

SAMCAR calculates the sums

$$S(IR,IE,IT) = \sum_{IA=1}^{NOA} F(IR,IE,IT,IA)$$

$$SQ(IR,IE,IT) = \sum_{IA=1}^{NOA} (F(IR,IE,IT,IA))^2$$

---

* The "effective" volume of a point detector is unity.

the relative statistical errors

$$\sigma(IR,IE,IT) = \frac{NOA}{S(IR,IE,IT)} \cdot \left\langle \frac{1}{NOA-1} \left\{ \left(\frac{SQ(IR,IE,IT)}{NOA} \right) - \left(\frac{S(IR,IE,IT)}{NOA} \right)^2 \right\} \right\rangle^{1/2}$$

and the average fluxes

$$\phi(IR,IE,IT) = \frac{S(IR,IE,IT)}{NHIST \cdot V(IR) \cdot \Delta E(IE) \cdot \Delta T(IT)}$$

where V(IR) is the volume* of scoring region IR, $\Delta E(IE)$ and $\Delta T(IT)$ are the widths of the energy and time bins.

The relative statistical errors are multiplied by 100 and are quoted in percent.

6.3 Description of Input Data for Program SAMOUT

Item 1 - Title Card, 80 columns of Hollerith (Format 20A4)

Item 2 - 20 Available Control Switches (Format 20I2)

KSWTCH(1) = 0 Statistical tape NAGG has been written

= 1 statistical tape IAGG must be processed and NAGG to be written

KSWTCH(2) = N N = number of response functions to be read.

(Response functions of unity are built in as a default option;
N=0 if this is the only response function.

If NAGG has been made on a previous run, this switch is ignored.)

KSWTCH(3) = 0 Edit all problems.

= 1 Omit this edit.

KSWTCH(4) = 0 Edit all problems summed over time.

= 1 Omit this edit.

---

* For a point detector, the volume is internally set to unity.

KSWTCH(5) = 0 Edit all problems summed with response functions.

= 1 Omit this edit.

KSWTCH(6) = 0 Edit all problems with response functions summed over time.

= 1 Omit this edit.

KSWTCH(7) = N Number of problem differences required for this run.

KSWTCH(8-11) = 0 or 1 Same as for KSWTCH(3-6) except here applied to required problem differences.

KSWTCH(15-16) = 0 No intermediate printout (for normal usage)

= 1 Print intermediate results

If KSWTCH(2) = 0 or KSWTCH(1) = 0, omit next item 3 and go to item 4 directly.

Item 3 - If KSWTCH(2)≠0 and KSWTCH(1) = 1 only: (Format 4E20.8)

Read prescribed list of response functions. Each new response function should start on a new card.

If KSWTCH(7) = 0, end of input; otherwise read in item 4.

Item 4 - Prescribed list of problem differences (Format 20I4)

e.g. if problem differences between problem 2 and 4, and between problem 5 and 7 are required, this card will read from columns 1-8 the following: 02040507.

End of Data.

6.4 Tape Utilization

The following describes the function of each tape used in the program. Tape numbers refer to Fortran logical numbers. All tapes are used in the binary mode.

Tape 1

The IAGG tape, the statistical aggregate tape from the previous program, SAMCAR, (denoted as TAPE 16 in SAMCAR).

Tape 2

A temporary storage tape while writing the NAGG tape.

Tape 3

A temporary storage tape while writing the NAGG tape.

Tape 4

The NAGG tape, the cumulative statistical tape from which all editing will be done.

7. PROGRAM SAMGAM: SECONDARY GAMMA PRE-PROCESSOR

7.1 General Discussion

Program SAMGAM is the data processing link of the SAMCEP system that couples a primary neutron transport solution to its corresponding secondary gamma transport solution. The data processing involves the generation or modification of three data files required for the secondary gamma transport: (1) an organized (i.e., "BAND FORMAT") gamma data tape (GODT), generated from a gamma element data tape (GEDT) produced by SAM-X; (2) a perturbation data tape (PDT), originally produced by SAMIN, modified by SAMSAM, and again modified by SAMGAM, so as to retain only concentration perturbations (the only "neutron" perturbations relevant to the secondary gamma transport); (3) an external source tape (EST) produced from a neutron interaction file (generated in the primary neutron transport) and a gamma production data tape (produced by SAM-X).

The generation of the GODT and PDT is performed by the BANDG and PREP8 routines, respectively, as described in Section 7.3. The EST is generated by the SAMSOU module (i.e., set of routines governed by SAMSOU), which, being the principal component of SAMGAM, is detailed in the following section. Flow charts for the SAMGAM program and the SAMSOU module are given in Figures 7.1 and 7.2, respectively.

7.2 The SAMSOU Module

The purpose of this module is to generate from a neutron interaction file (IF, output of SAMCAR) and a gamma production data tape (GPDT), the external source tape (EST) required by SAMCAR for secondary gamma transport.

Each neutron interaction represents a non-elastic event for each of up to ten correlated problems. The information distinguishing any one problem from all the others is a weight which is the cumulative product of the weights due to the relevant perturbations over the history leading to the event. In

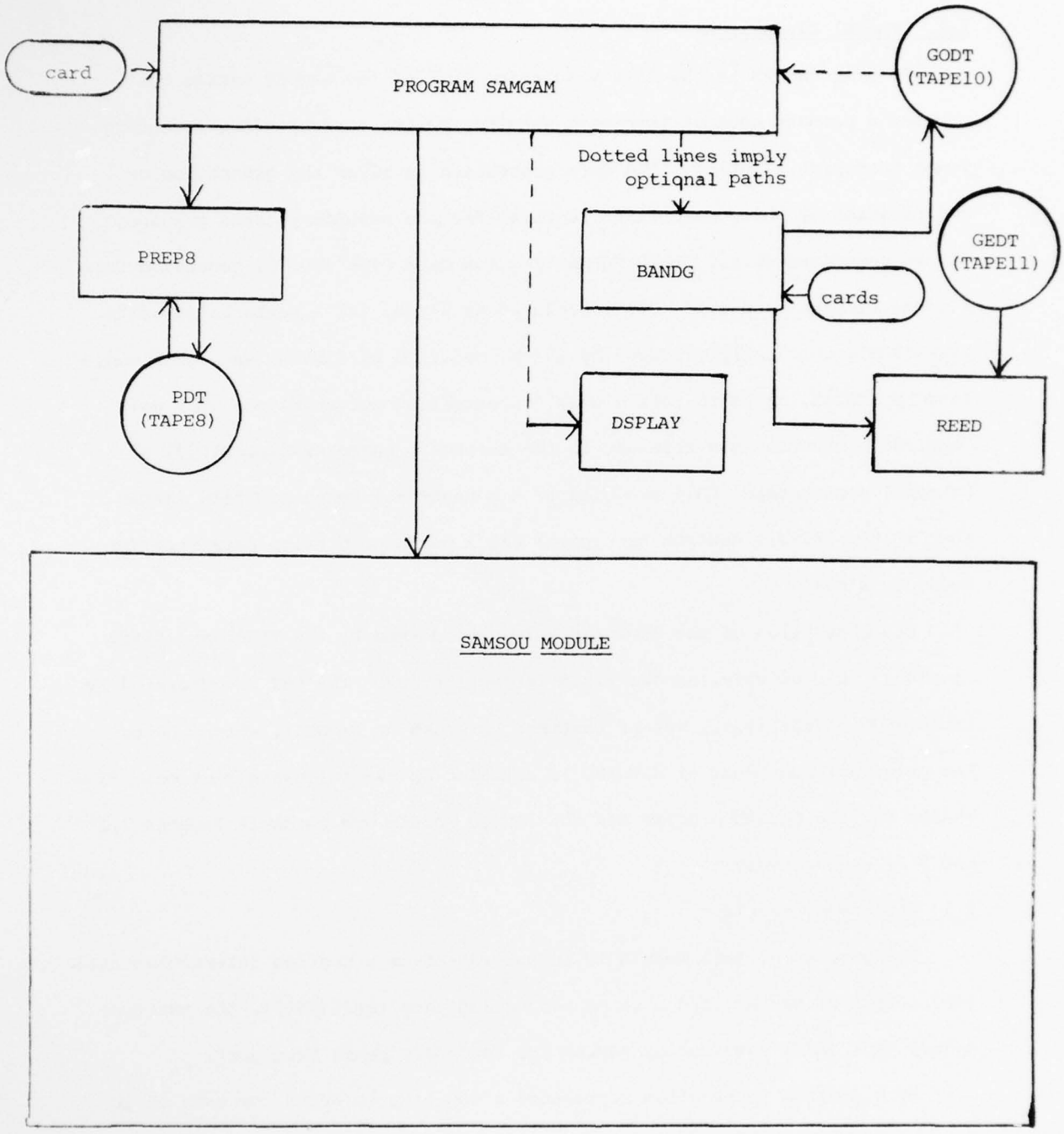

FIGURE 7.1 - Flow Chart for SAMGAM Program

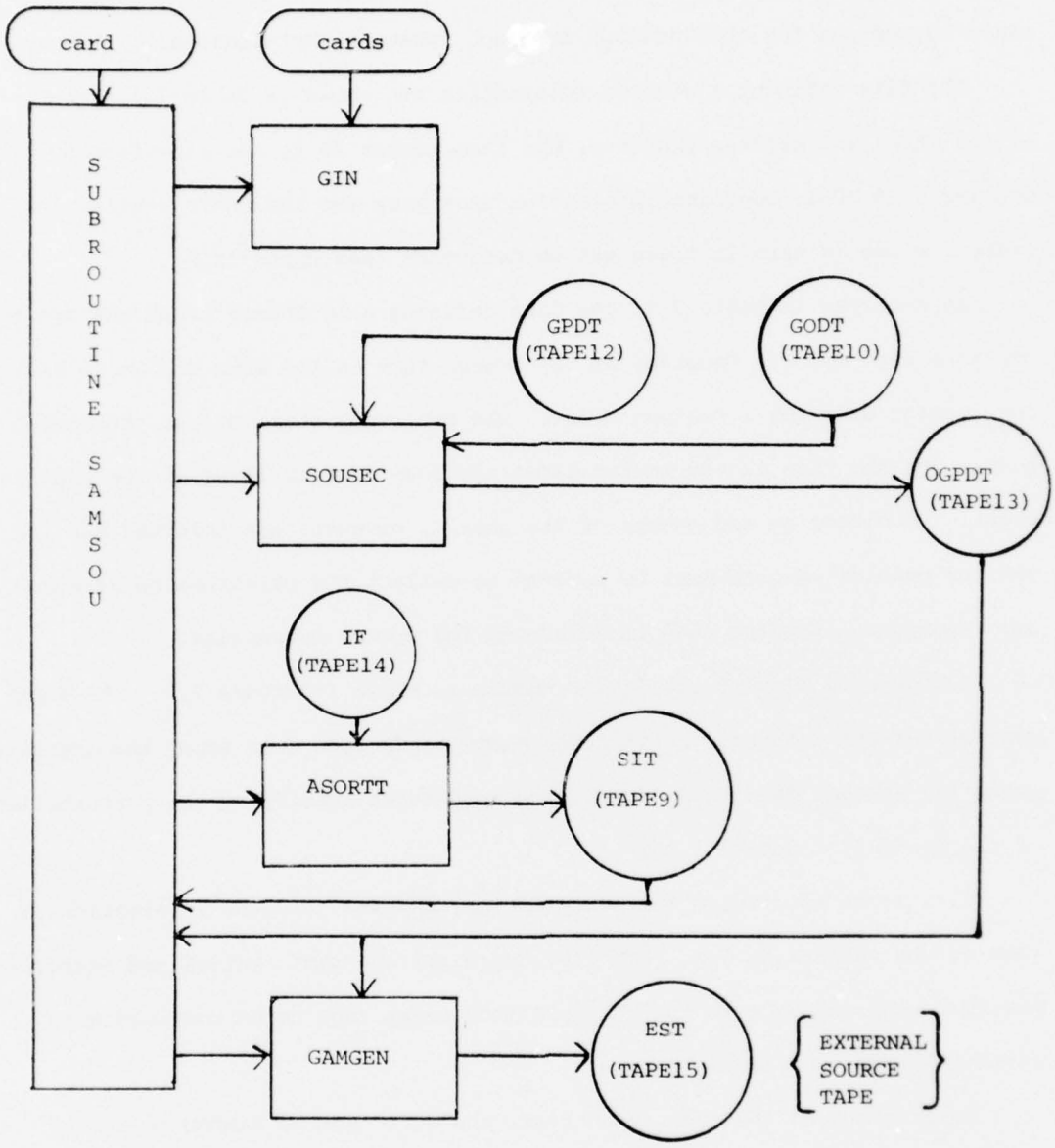

FIGURE 7.2 - Flow Chart for SAMSOU Module

accordance with this, a given output problem may also be made the subject of perturbations in the gamma production data by updating the secondary gamma ray weight for that problem for each relevant perturbation.

The data defining a neutron interaction are shown in Table 7.1. Most of the items are self-explanatory, but item number 10 may be clarified by stating that KDLIV contains information necessary for the angle reselection procedure and is zero if there are no detectors (see Appendix F).

As depicted in Table 7.1, the data defining a secondary gamma ray are of the same type and are recorded on the source tape in the same format as the interaction data for a neutron event. The cartesian coordinates, the region number and the time of the source gamma are identical to those of the neutron event. The direction and energy of the photon, however, are selected and the various problem weights must be updated to reflect the perturbation data and any importance sampling used in selecting the photon properties.

The general flow of the SAMSOU module is shown in Figure 7.2. The input consists of the interaction file, the gamma production data tape, the organized gamma ray element data tape (GODT), and card input specifying the perturbations of the production data (if any).

Card input specifying the perturbations and the detector information is read by the subroutine GIN. GIN also organizes the perturbation and energy importance sampling data in the MISTER-SISTER array (not to be confused with identically named array in SAMCAR).

After the card input has been read, the next task of SAMSOU is to reorganize the GPDT so that only those elements occurring in the problem are represented on the organized gamma production data tape (OGPDT). This reorganization is accomplished by a call to subroutine SOUSEC, which utilizes information from the gamma ray element data tape (GODT) to select the elements and establish the order of occurrence.

The next task, accomplished through a call to subroutine ASORTT, is to sort each statistical group of interactions on the IF so that the element order within a group corresponds to that on the OGPDT. The output of this operation is a sorted interaction tape (SIT).

The main calculational routine of this module is GAMGEN. This routine operates on a full buffer of interactions (35) to produce the required number of secondary gamma rays, as given on input. A buffer of 35 secondary rays is written onto the source tape as soon as it is filled.

Two types of perturbations of gamma production data are permitted: 1) perturbation of yield (multiplicity) data for specified photons from specified elements interacting with neutrons in specified energy ranges and 2) perturbation of angular distribution data for specified photons from specified elements in collision with neutrons in specified energy ranges.

In addition to allowing for perturbation of the gamma production data, SAMSOU allows for the selection of the photon from an alternative yield set, thus providing for energy importance sampling. The alternative yield set is input as a quadratic function of gamma energy from which discrete relative yield values are obtained for the given photon energies.

The secondary gamma ray directions which are recorded on the source tape are subjected to the reselection procedure, required by the bounded flux-at-a-point (BFAP) procedure, in GAMGEN. Hence, the role of the OGPDT terminates with the completion of the source tape.

7.3 Description of Routines

This section gives a brief description of the routines which comprise the SAMGAM program. The routines are presented in the order in which they are invoked:

ROUTINE	DESCRIPTION
SAMGAM	This is the main program. Its principal function is to direct the processing of the three data files: GODT, PDT, and EST. It reads one input card, which specifies whether or not the GODT is available from a previous execution of BANDG. It also establishes the length of blank common and initializes certain flags.
BANDG	This subroutine is called by SAMGAM if a GODT has not previously been prepared. It is a simplified version of the BAND routine of program SAMSAM. The GODT is generated in one energy band.
REED	This utility routine provides the calling routine (BANDG) with the flexibility of effecting an unformatted read of a complete array, whose dimension is an argument of the call. This obviates the use of an implied loop in the FORTRAN supplied READ utility, which is slower.
DSPLAY	This utility routine accepts as arguments the first member of a sequence in memory, and the desired number of consecutive entries to be displayed. It then prints out the specified set of entries, up to ten per line, with an internally computed cumulative count as an eleventh printed integer. It automatically discriminates between fixed and floating point entries, and uses either I12 or E12.4 format, respectively.
PREP8	This routine, called by SAMGAM, modifies the PDT as follows: every entry of the NTYP array (see Section 3.1) is set equal to NTYP(1), the INBAND array (see Section 4.1) is zeroed out, and the value of KEGEOM (see Section 4.3) is made to correspond to the GODT. The PDT is then overwritten on TAPE8.
SAMSOU	The governing routine for the external source generating module, SAMSOU is called from SAMGAM after the GODT has been produced. SAMSOU reads one card of data directly: NSTOP, the number of precursor histories, NSTAT the number of such histories per statistical group, and NGAM, the desired number of gamma ray histories. The rest of the card input is then read by GIN, the first subroutine called by SAMSOU. SAMSOU then calls the tape organizing routines SOUSEC and ASORTT. After ASORTT has returned the total number of interactions on the SIT, SAMSOU calculates an integer, NFACT, and a real number, SFACT < 1.0, such that the sum represents the average number of gammas to be produced from each interaction. Then SAMSOU reads in buffers of 35 interactions from the SIT and calls GAMGEN to process each buffer.

ROUTINE	DESCRIPTION
GIN	This subroutine, the first called from SAMSOU, reads the rest of the card input, and locates data for the perturbations in the MISTER-SISTER array, creating pointers as it reads and stores. The data read by GIN also includes energy importance sampling parameters and detector information. The detector information required is, for each detector, the position coordinates, the radius of the critical sphere, the physical region and the overlap index. After all of the data have been read, GIN prints it out in an easily read format.
SOUSEC	The third routine called by SAMSOU, SOUSEC is responsible for organizing the gamma production data tape. For this, SOUSEC needs the header information from the GODT, specifically the identification of elements in the problem. SOUSEC searches the GPDT for the data for each element and writes the data on the OGPDT as two logical records. The first is simply the length (LENGTH) of the data record. The organization of the second, or data, record may be found in Appendix D of the SAM-CE manual, starting with word number 3 (the first two words are deleted for the OGPDT). The pointers for the data are adjusted to reflect the known starting location in the MISTER array, which is supplied by GIN. SOUSEC leaves resident in memory the ordered array of element identifiers. The only other output is the OGPDT.
ASORTT	The function of this routine is to reorder the interactions within each statistical group according to the element involved in the interaction. ASORTT also counts the number of interactions on the tape (NINT) for use in computing the number of gamma rays to be produced for each interaction. The input to ASORTT is the IF. Other required information is the ordered array of element identifiers. The output is the sorted interaction tape SIT.

ROUTINE	DESCRIPTION
GAMGEN	GAMGEN (IFLAG) is the main calculational routine of this module. This routine treats a complete buffer of 35 interactions, producing as many gamma rays per interaction as required by input. For each gamma ray an energy (one of a discrete set) and a direction must be selected. The data for these selections are read into the MISTER-SISTER array from the OGPDT for a given element and remain there until the interactions for that element are exhausted. The photon energy may be selected from the true yield data or from an alternative set, with appropriate weighting. The alternative set is calculated for each event from a user-supplied quadratic function of photon energy, the same for all neutron energies. Thus some energy importance sampling is available. The initial direction selection is based on the data from the OGPDT and then, if detectors are present, angle re-selection with the indicated re-weighting, is effected by a call to subroutine ARG. After the energy and angle selections are complete, GAMGEN examines each perturbation in turn to determine whether it applies to this element, this photon, and this neutron energy. The additional weight factor is computed for each relevant perturbation and multiplies the weight of each output problem to which the perturbation applies. GAMGEN writes buffers of 35 gamma rays onto the source tape. Other routines called by GAMGEN are DIREC, RANF, SEEK, and ARG, which calls ARPREP. These are described elsewhere.

7.4 Card Input Formats

This section describes the card input required for executing the SAMGAM program. The input formats are presented in two sections, for clarity, but are understood to represent one contiguous data record. The two sections deal with generation of the GODT and the EST, in that order.

7.4.1 Input Formats for GODT Generation

Card 1: Format (2I5) (read by SAMGAM)

KEGEOM	Zero (or blank) if generation of GODT ("banding") is required; otherwise, the value of KEGEOM, as printed out in the previously generated GODT run.
IDBG	A positive integer value will cause the GODT to be displayed.

If KEGEOM is given as a positive integer, the remainder of the input described in this sub-section is bypassed (i.e., proceed with Section 7.4.2). Otherwise, the following cards are read by BANDG.

Card 2: Format (3I10)

NO	Arbitrary run identifier.
NCOMP	Number of compositions.
NG	Unity for gamma cross sections.

For each of the NCOMP compositions, the following sets of cards are required:

Card(s) 3: Format (I10)

NE	Number of elements for this composition.

For each of the NE elements, one card of the following form is required:

Card(s) 4: Format (2I10, E15.6)

IT	Arbitrary counter.
ID	Element identifier (ZZAAA)
CONC	Atomic concentration given in units of (10^{24} atoms/cm^3)

The SAMGAM input continues with the card formats described in the section that follows.

7.4.2 Input Formats for Gamma Ray Source Generation

Card 1: Format (4I10) (read by SAMSOU)

NSTOP	number of precursor neutron histories
NSTAT	number of precursor histories per statistical group
NGAM	total number of gamma histories to be run; default (if left blank) leaves decision up to gamma production data;
NAGG	number of aggregates to be used in a preliminary computation of the multiplicative factor which will produce the desired NGAM. Default (if left blank) is 1.

Card 2: Format (3I5)

KK1	number of perturbations of type 1
KK2	total number of perturbations (type 1 + type 2)

Cards 3 through 8 are needed only if KK2>0.

Card 3: Format (14I5)

Start new card for each perturbation:

IP	perturbation type (1 or 2)
NPROB	number of output problems affected
JPROB(1)	ordinal number of first affected problem
.	
.	
.	
JPROB(NPROB)	ordinal number of last affected problem

The rest of the cards are grouped by perturbation. For both perturbation types:

Card 4: Format (14I5)

ID	element identifier
NPH	number of photons affected
JPH(1)	ordinal number of first photon
.	
.	
.	
JPH(NPH)	ordinal number of last photon

Card 5: Format (I5,2E15.5)

NEP — number of neutron energies

EHIGH — highest neutron energy

ELOW — lowest neutron energy

Card 6: Format (5E15.5)

(EN(I),I=1,NEP) — neutron energies for which perturbation data are tabulated. EN(1)>EHIGH EN(NEP)<ELOW.

For perturbations of type 1:

Card 7: Format (5E15.5) (NEP sets)

(Y(1,J),J=1,NPH) — yields for EN(1) for each photon

.
.
.

(Y(NEP,J),J=1,NPH) — yields for EN(NEP) for each photon

NOTE: Start new card for each energy point.

For perturbations of type 2:

Card 7: Format (14I5)

(NX(I),I=1,NEP) — number of CHI values for each energy EN(I)

Card 8: Format (5E15.5) (NEP sets)

(CHI(1,J),J=1,NX(1)) CHI values for EN(1)

.
.
.

(CHI(NEP,J),J=1,NX(NEP) CHI values for EN(NEP)

NOTE: Endpoint values (0.0 and 1.0) are not to be given in the CHI-sets.

Card 9: Format (3E15.5)

A, B, C — Coefficients in the quadratic formula for alternative yield data: $(Y(E_I)=AE_I^2 + BE_I + C.$ Can be used to obtain some energy weighting. For no energy importance enter (0.0,0.0,1.0).

Card 10: Format (I5)

NDET — Number of detectors.

For each of the NDET detectors:

Card 11: Format (4E15.5,2I5)

XAD, YAD, ZAD — x, y and z coordinates for this detector.

CRAD — radius of the critical sphere for this detector, output of the neutron problem.

IRDET — physical region of this detector, output of the neutron problem.

LAP — signal indicating either the absence (0) or the presence (1) of overlays of the critical sphere of this detector with that of any other detector. Also an output of the neutron problem.

Table 7.1 The Twenty-Four Word Array Defining a Non-elastic Event and the Equivalent Array Defining a Secondary Source

Word(s)	Name	Description		
		Non-elastic Event		Secondary Gamma
1-3	$\overline{XB}$	Cartesian Coordinates of event	≡	Cartesian coordinates of Gamma
4-6	$\overline{WB}$	Direction of precursor primary particle		Direction selected for Gamma
7	E	Energy of precursor primary particle		Energy of selected Gamma
8	IR	Region number	≡	Region number
9	T	Time of event	≡	Time of origin
10	IDET	200000*KDLIV +SIGN(KDLIV)*IATWT	≡	Same
11	F	Ignored		Ignored
12	NHIST	Primary Particle History number		Same
13	W	Ignored		Ignored
14	J12345	10		10
15	WT(1)	Weight for Problem 1		Updated Weight for Problem 1
16	WT(2)	Weight for Problem 2		Updated Weight for Problem 2
.	.	.		
.	.	.		
.	.	.		
24	WT(10)	Weight for Problem 10		Updated Weight for Problem 10

7.5 Organization of the MISTER-SISTER Array

(This array is independent of the identically named array in the SAMCAR program).

LOCATION	CONTENTS	REMARKS
1	LN1	Location of NPROB for perturbation 1
.	.	.
.	.	.
KK	LNKK	Location of NPROB for perturbation KK
.	.	.
.	.	.
KK2	LNKK2	Location of NPROB for perturbation KK2
KK2+1	LOCD	Location of last output problem number for last perturbation
KK2+2=LN1	NPROB	(NPROB for first perturbation)
KK2+3	JPROB(1)	first output problem number for first perturbation
.	.	.
.	.	.
KK2+2+I	JPROB(I)	Ith output problem number for first perturbation
.	.	.
.	.	.
KK2+2+NPROB	JPROB(NPROB)	last output problem number for first perturbation
(Bracketed sequence repeated for each perturbation)		
.	.	.
LOCD+1	LOC1	location of first data word for first perturbation
.	.	.
.	.	.
LOCD+I	LOCI	location of first data word for Ith perturbation
.	.	.
.	.	.
LOCD+KK2	LOCKK2	location of first data word for last perturbation
LOCD+KK2+1	LOCIMP	location of first coefficient of importance function

(Following sequence for each perturbation in order)

LOCATION	CONTENTS	REMARKS
LOCI+1	ID	element ID for Ith perturbation
LOCI+2	NPH	number of photons affected
LOCI+3	JPH(1)	ordinal number-first photon
.	.	.
.	.	.
LOCI+2+J	JPH(J)	ordinal number-Jth photon
.	.	.
.	.	.
LOCI+2+NPH	JPH(NPH)	ordinal number-last photon
LOCI+NPH+3	NEP	number of energies in neutron table
LOCI+NPH+4	EHIGH	high energy limit
LOCI+NPH+5	ELOW	low energy limit
LOCI+NPH+6	----	blank
LOCI+NPH+7	EN(1)	first energy, neutron table
.	.	.
.	.	.
LOCI+NPH+6+J	EN(J)	Jth energy, neutron table
.	.	.
.	.	.
LOCI+NPH+6+NEP	EN(NEP)	last energy, neutron table

NOTE: the sequences for the two types of perturbation diverge here. Let LOCIP=LOCI+NPH+6+NEP.

For Type 1:

LOCIP+1	Y(1,1)	yield for photon JPH(1) at EN(1)
.	.	.
.	.	.
LOCIP+NPH	Y(1,NPH)	yield for photon JPH(NPH) at EN(1)
.	.	.
	.	.
	.	.
LOCIP+NEP*NPH+1	Y(NEP,1)	yield for photon JPH(1) at EN(NEP)
.	.	.
	.	.
LOCIP+(NEP+1)*NPH	Y(NEP,NPH)	yield for photon JPH(NPH) at EN(NEP)

For type 2:

LOCATION	CONTENTS	REMARKS
LOCIP+1	NX(1)	number of CHI values at EN(1)
◦	•	•
•	•	•
LOCIP+NEP	NX(NEP)	number of CHI values at EN(NEP)
LOCIP+NEP+1	CHI(1,1)	CHI-1 at energy EN(10)
•	•	◦
•	◦	•
LOCIP+NEP+NX(1)	CHI(1,NX(1))	CHI-NX(1) at energy EN(1)
•	•	•
•	•	•
LOCIP+NEP+$\sum_{J=1}^{NEP-1}$ NX(J)+1	CHI(NEP,1)	CHI-1 at energy EN(NEP)
◦	•	•
•	◦	•
LOCIP+NEP+$\sum_{J=1}^{NEP}$ NX(J)	CHI(NEP,NX(NEP))	CHI-NX(NEP) at EN(NEP)
LOCIMP	A	coefficient of square of photon energy
LOCIMP+1	B	coefficient of photon energy
LOCIMP+2=LOCEL	C	constant

NOTE:A,B,C are used to compute alternate yield data (relative yields).

LOCEL+1	ID	element identifier - start of gamma production data

7.6 Tape Utilization

The following describes the function of each tape used in the program. Tape numbers refer to FORTRAN logical numbers. All tapes are used in the binary mode.

Tape 8

This is the perturbation data tape (PDT), generated by SAMIN, then modified by SAMSAM and by SAMGAM (retaining only concentration perturbations, if any).

Tape 10

This is the organized data tape for gammas (GODT) generated by SAMGAM.

Tape 11

This is the gamma element data tape (GEDT) generated by SAM-X, from which the GODT is generated.

Tape 12

This is the gamma production data tape (GPDT) generated by SAM-X.

Tape 14

This is the neutron interaction file (IF) generated in the primary neutron run by SAMCAR.

Tape 15

This is the external source tape (EST) produced by SAMGAM.

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2. M. K. Drake (ed.), "Data Formats and Procedures for the ENDF Neutron Cross Section Library", BNL 50274/ENDF 102, Vol. 1 (Oct. 1970).

3. H. A. Steinberg and M. H. Kalos, "Bounded Estimators for Flux-at-a-Point in Monte Carlo", Nuc. Sci. and Eng.:44, 406-412 (1971).

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5. H. A. Steinberg, "Bounded Estimation of Flux-at-a-Point for One or More Detectors", ANL-NEACRP Meeting of a Monte Carlo Study Group, Argonne National Laboratory (July 1974).

APPENDIX A

THE COMBINATORIAL GEOMETRY TECHNIQUE FOR THE DESCRIPTION AND COMPUTER PROCESSING OF COMPLEX THREE-DIMENSIONAL OBJECTS

A.1 Introduction

Combinatorial Geometry is essentially a technique for representing, in a computer, a mathematical model of a three-dimensional geometric configuration. Once in the computer, the configuration can be analyzed in many different ways by ray-tracing techniques. For example, quantities such as volumes, surface areas, object boundaries, line of sight distances, etc. are readily determined. Regardless of the application, however, the basic concepts employed are the same. A discussion of these concepts can logically be broken down into two topics. That is, geometry description and ray-tracing, which are discussed separately below.

A.2 Description of the Combinatorial Geometry Technique

In order to perform computer studies concerning a complex three-dimensional object one must first be able to prepare a mathematical model of the object and its environment. The combinatorial geometry technique has been developed to permit a model to be produced which is both accurate and suitable for a ray-tracing analysis program. The latter feature is important since nuclear radiation analysis by Monte Carlo involves the tracing of rays through geometrical models.

In effect the geometric description subdivides the problem space into unique regions. This is achieved through the use of ten specific geometric bodies (closed surfaces) and the orderly identification of the combination of these bodies to define a region (space volume). The bodies which will be discussed further in INPUT Preparation (Section A.2.2) are as follows:

1. Rectangular Parallelepiped (RPP)
2. Box
3. Sphere
4. Right Circular Cylinder
5. Right Elliptical Cylinder
6. Truncated Right Angle Cone
7. Ellipsoid of Revolution
8. Right Angle Wedge
9. Arbitrary Convex Polyhedron of four, five or six sides (each side having three or four vertices)
10. Truncated Elliptical Cone

Except for the RPP's, all bodies may be arbitrarily oriented with respect to the x, y, z coordinate axes used to determine the space. It should be noted that the sides of an RPP must be parallel to the coordinate axes.

A.2.1 Region Description Technique

The basic technique for the description of the geometry consists of defining the location and shape of the various physical regions (wall, equipment, etc.) in terms of the intersections and unions of the volumes contained in a set of simple bodies. A special operator notation involving the symbols (+), (-), and (OR) is used to describe the intersections and unions. These symbols are used by the program to construct tables used in the ray-tracing portion of the problem.

If a body appears in a region description with a (+) operator, it means that the region being described is wholly contained in the body.

If a body appears in a region description with a (-) operator, it means that the region being described is wholly outside the body.

The (OR) operator is used to form regions as unions of subregions, where each subregion is defined in terms of one or more bodies, using (+) or (-) as described above. Then a point is in the region if it is in any subregion.

The technique of describing a physical region is best illustrated by an example. Consider an object composed of a sphere into which is inserted a cylinder. This is shown in cross section in Figure A.2.1(a).

To describe the object, we take a spherical body penetrated by a cylindrical body (Figure A.2.1(b)). Each body is numbered. Consider the sphere as body No. 1 and cylinder as body No. 2. If the materials in the sphere and cylinder are the same, then they can be considered as one physical region, say region 100 (Figure A.2.1(c)).

The description of region 100 would be

100 = (OR 1) (OR 2).

This means that a point is in region 100 if it is <u>either</u> inside body 1 <u>or</u> inside body 2.

If different materials are used in the sphere and cylinder, then the sphere with a cylindrical hole in it would be given a different region number (say 200) from that of the cylinder (300).

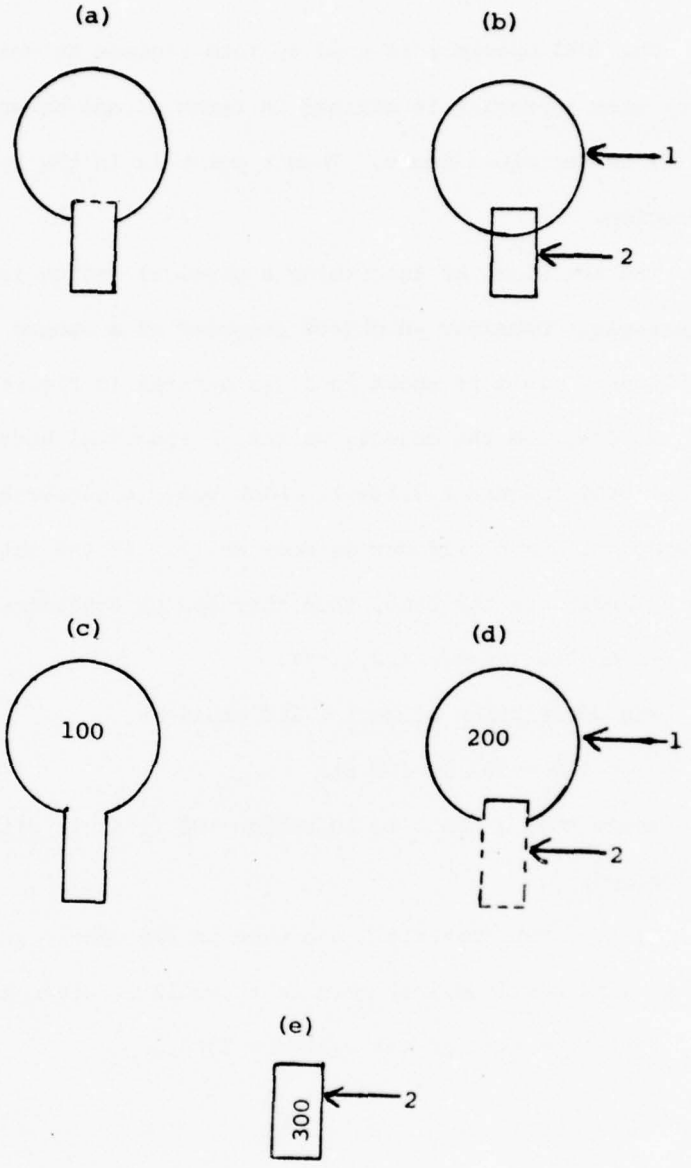


Figure A.2.1 - Regions Produced by Intersections and Unions of Sphere and Cylinder

The description of region 200 would be (Figure A.2.1(d))

200 = (+1) (-2).

This means that points in region 200 are all those points inside body 1 which are not inside body 2.

The description of region 300 is simple (Figure A.2.1(e))

300 = (+2)

That is, all points in region 300 lie inside body 2.

This technique, of course, can be applied to combinations of more than two bodies and such region descriptions could conceivably contain a long string of (+), (-) and (OR) operators. The important thing to remember is that every spatial point in the geometry must be located in one and only one region. Further examples are given in Section A.2.2.2.

The user of the program will specify the geometry by establishing two tables. The first table will describe the type and location of the set of bodies used in the geometrical description. The second table will identify the physical region in terms of these bodies. The computer program processes these tables to put the data in the form required for ray tracing. All of the space must be divided into regions, and once again, no point may be in more than one region.

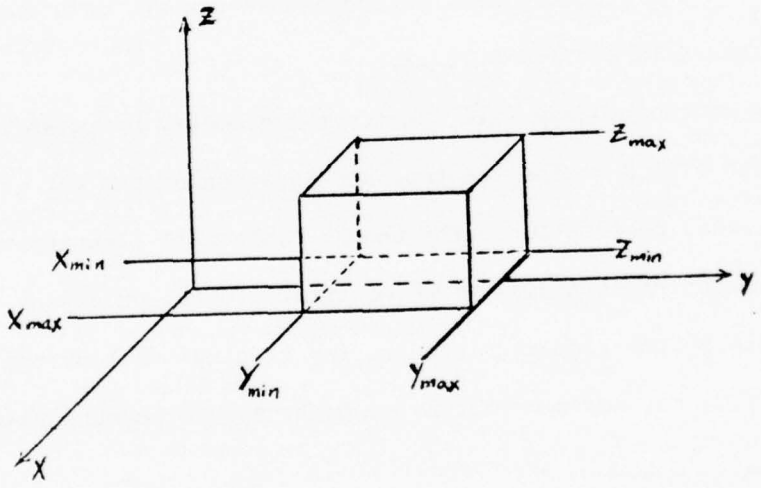
A.2.2 Input Preparation

A.2.2.1 Description of Input Parameters

The information required to specify each type of body is as follows.

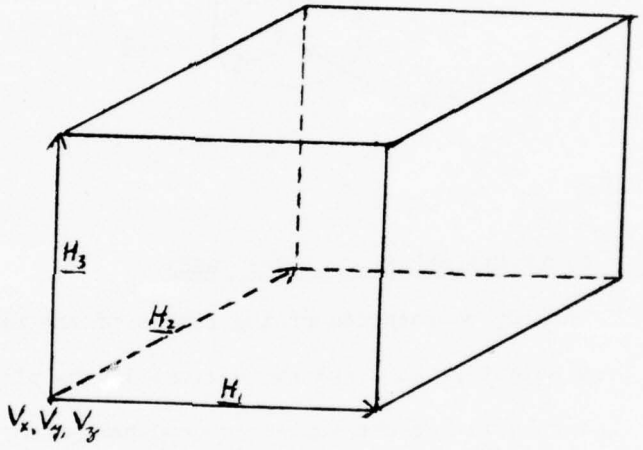
1. Rectangular Parallelepiped (RPP)

These bodies are used for gross subdivisions of the geometry and must have bounding surfaces parallel to the coordinate axes. Specify the maximum and minimum values of the x, y, and z coordinates which bound the parallelepiped.



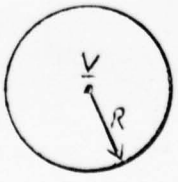
2. Box (BOX)

Specify the vertex $\underline{V}$ at one of the corners by giving its (x,y,z) coordinates. Specify a set of three mutually perpendicular vectors, $\underline{H}_i$, representing the height, width, and length of the box, respectively. That is, the x,y, and z components of the height, width, and length vectors are given.



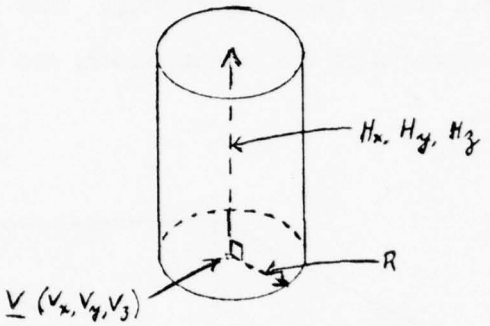
3. Sphere (SPH)

Specify the vertex $\underline{V}$ at the center and the scalar, R, denoting the radius.



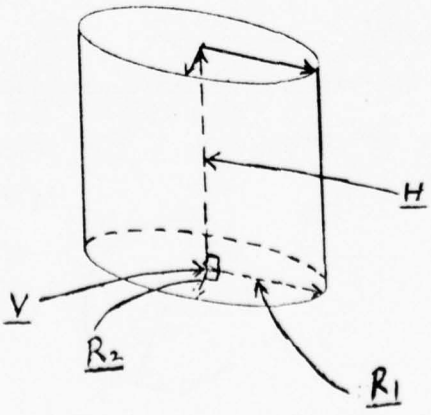
4. Right Circular Cylinder (RCC)

Specify the vertex $\underline{V}$ at the center of one base, a height vector, $\underline{H}$, expressed in terms of its x, y, and z components, and a scalar, R, denoting the base radius.



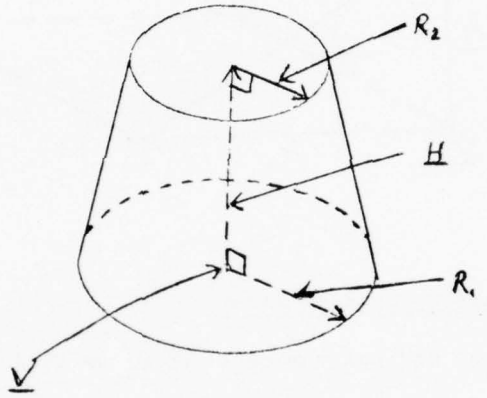
5. Right Elliptical Cylinder (REC)

Specify coordinates of the center of the base ellipse, a height vector, and two vectors in the plane of the base defining the semi-major and semi-minor axes, respectively.



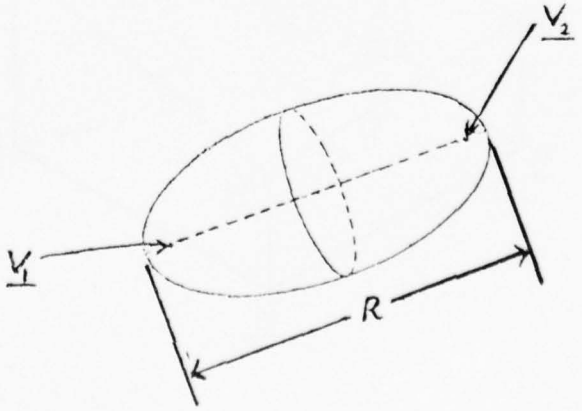
6. Truncated Right Angle Cone (TRC)

Specify a vertex $\underline{V}$ at the center of the lower base, the height vector, $\underline{H}$, expressed in terms of its x, y, z components, and two scalars, R_1 and R_2, denoting the radii of the lower and upper bases.



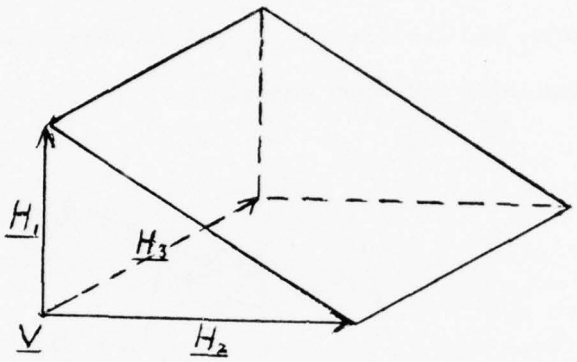
7. Ellipsoid (ELL)

Specify two vertices, $\underline{V_i}$, denoting the coordinates of the foci and scalar, R, denoting the length of the major axis.



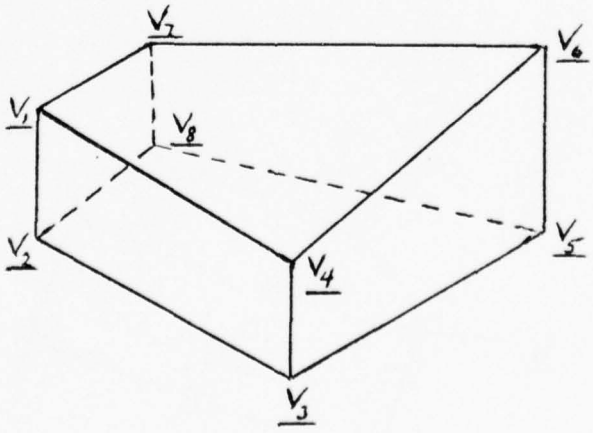
8. Right Angle Wedge (RAW)

Same input as for the boxes. However, H_1 and H_2 describe the two legs of the right triangle of the wedge.



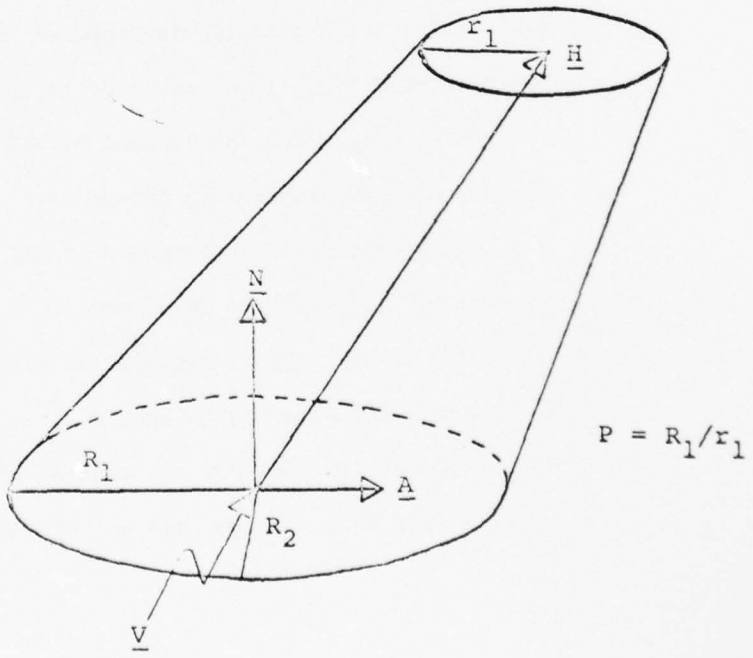
9. Arbitrary Polyhedron (ARB)

Assign an ordinal number (1 to 8) to each vertex. For each vertex, give the x,y,z coordinates. For each side of the figure list the ordinal vertex numbers. The vertices and side descriptions may be given in any order. An example is given later.



10. Truncated Elliptical Cone (TEC)

Specify the coordinates of the vertex V at the center of the larger ellipse; the x,y, and z components of height vector H; the components of normal vector, N, directed inward at V; the components of direction vector, A, along major axis; the semi-major and semi-minor axes of larger ellipse, R_1 and R_2, respectively; the ratio, P, of the larger to the smaller ellipse axis. Note that direction vectors N and A are normalized internally (after input printout).



A.2.2.2 Examples of Region Descriptions

Some representative geometries and their input descriptions are shown below.

Example 1 - Two Spheres Within an RPP (See Figure 2.2)

The body input table is shown below.

TABLE I - BODY INPUT DESCRIPTION

Body	Type of Data Required
1	List the six bounding coordinate values (X_{min}, X_{max}, Y_{min}, Y_{max}, Z_{min}, Z_{max})
2	List the vertex and radius of sphere 2
3	List the vertex and radius of sphere 3

One possible region input table is shown below.

TABLE II - REGION DESCRIPTION

Region	Input
100	(+1) (-2) (-3) (Region 100 is composed of all points interior to RPP No. 1 and exterior to spheres 2 and 3)
200	(+3) (-2) (Region 200 is composed of all points interior to sphere 3 and exterior to sphere 2)
300	(+2) (+3) (Region 300 is composed of all points which are in sphere 2 and are also in sphere 3)
400	(+2) (-3) (Region 400 is composed of all points interior to sphere 2 and exterior to sphere 3)
500	(OR 2) (OR 3) (If desired, one region, the total of regions 200, 300, and 400, can be defined as region 500).

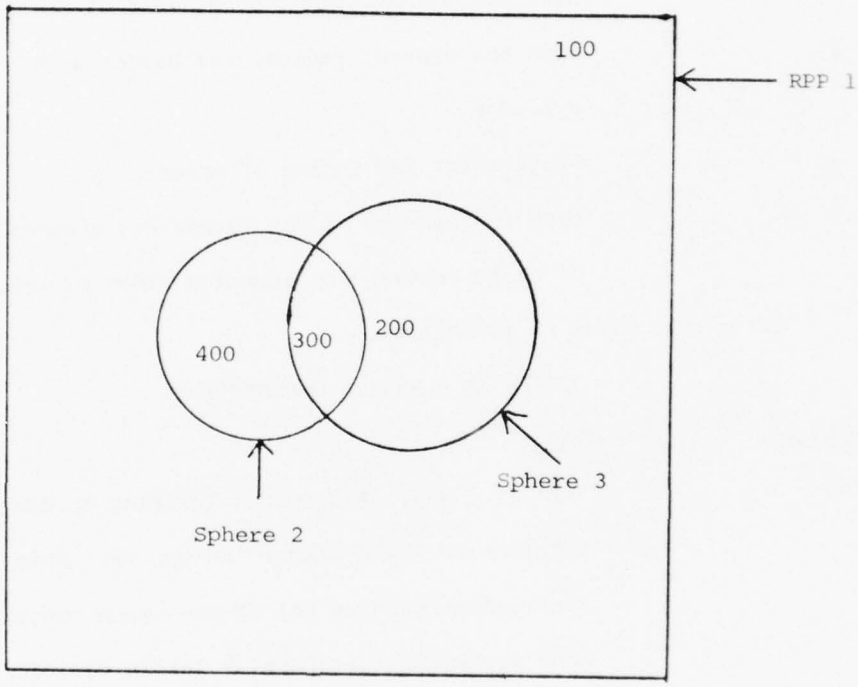


Figure A.2.2 - Regions Produced by Intersections and Unions of Two Spheres

Example 2 - Cylinder Divided into Two Regions by a Box and with a Sphere at One End (See Figure A.2.3)

TABLE I - BODY INPUT DESCRIPTION

Body	Type of Data Required
1	List the six bounding coordinates of the RPP
2	List the vertex, radius, and height vector of cylinder
3	List center and radius of sphere
4	List coordinates of one corner and components of three vectors representing sides of box.

The region input is as follows.

TABLE II - REGION DESCRIPTION

Region	Input
100	(+1) (-2) (-3) (All points interior to the RPP and exterior to the cylinder and sphere. Note that region 100 includes all of the space contained inside body 4, except that portion inside cylinder 2. This space can be assigned a special region number, if desired. If, as in this example, it is not desired, it is not necessary).
200	(+2) (-4) (All points interior to the cylinder, and outside the box).
300	(+3) (-2) (All points interior to the sphere and external to the cylinder).
400	(+2) (+4) (All points interior to the cylinder and also inside the box).

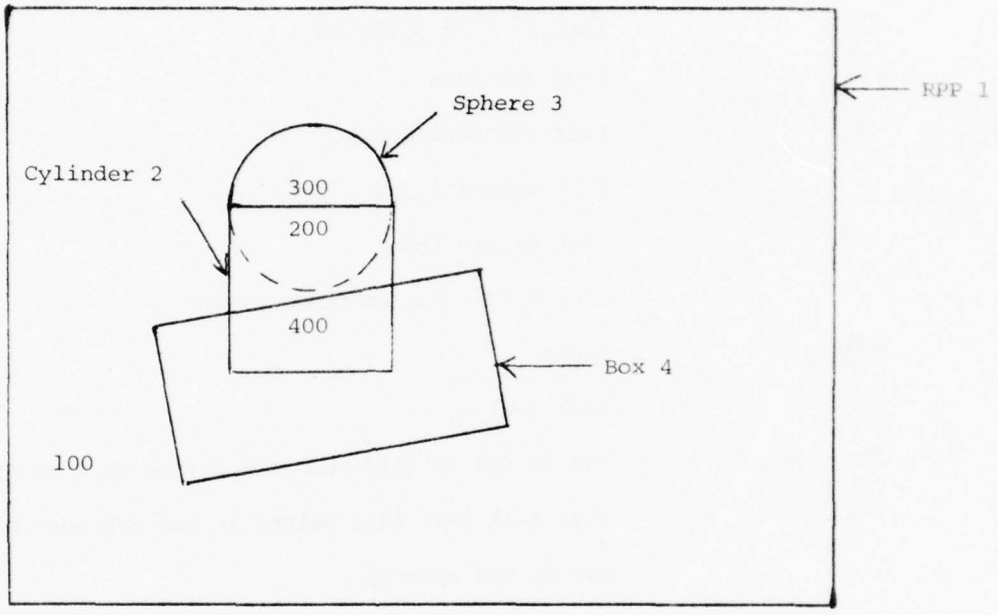


Figure A.2.3 - Regions Produced by Intersections and Unions of Sphere, Circular Cylinder, and Box

Example 3 - Multiple Region Capability - Cylinder Containing Two Spheres, All Inside an RPP (See Figure A.2.4)

TABLE I - BODY INPUT DESCRIPTION

Body	Type of Data Required
1	List RPP data
2	List cylinder input
3	List sphere input
4	List sphere input

TABLE II - REGION DESCRIPTION

Region	Input
100	(+1) (-2)
200	(OR 3) (OR 4) (All points interior to 3 or 4)
300	(+2) (-3) (-4) (All points in the cylinder but not in the spheres).

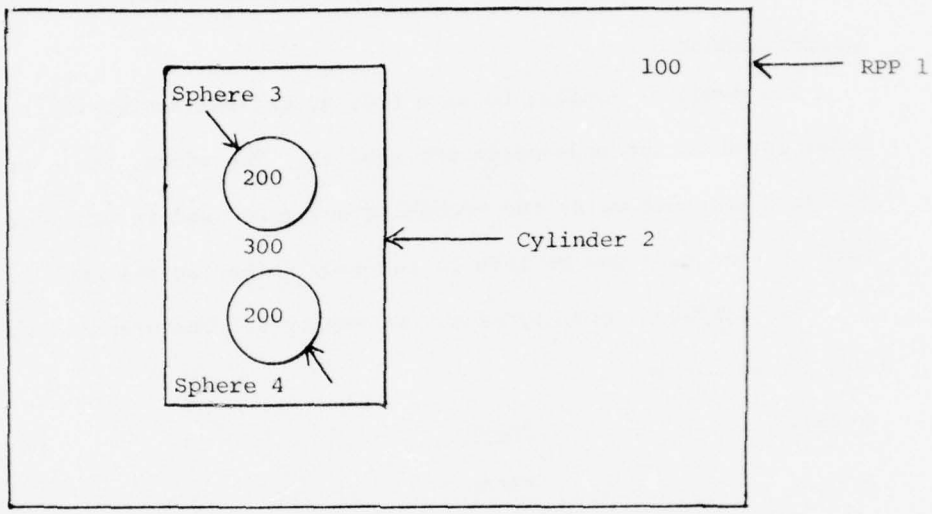


Figure A.2.4 - Example of Physical Region Produced from Unconnected Regions Using "OR" Statement

A.2.2.3 Card Input Formats

The following punched cards are needed to describe the geometry and must appear in the order in which they are described below.

1. Body Cards

The computer assigns to each body an ordinal number which depends on the order in which the body cards are read in. Therefore, it is most important that the card sequence match the numbering sequence used in the region descriptions. Note that no gaps may be left in the body numbering sequence.

Ten different body types may be employed. The standard format for each body is as follows:

Columns	Input
1-2	Blank
3-5	Three-letter body identifier
6	Blank
7-10	Four characters or arbitrary integer data
11-70	Divided into six floating point fields of 10 columns each. Body dimensions are given here.

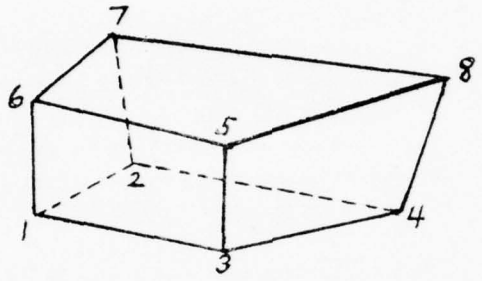
Table A.2.1 describes the input required for each body. The quantities V, H, etc., were defined in Section A.2.2.

Note that the last card of the body data must be END punched in columns 3,4,5. This is the signal that all body data have been treated.

TABLE A.2.1 - INPUT REQUIRED FOR EACH BODY TYPE

Body Type	3-letter ID	Card Columns 11-20	21-30	31-40	41-50	51-60	61-70	Number of Cards Needed
Rectangular Parallelepiped	RPP	X_{min}	X_{max}	Y_{min}	Y_{max}	Z_{min}	Z_{max}	1
Box	BOX	Vx	Vy	Vz	H1x	H1y	H1z	1 of 2
		H2x	H2y	H2z	H3x	H3y	H3z	2 of 2
Sphere	SPH	Vx	Vy	Vz	R	-	-	1
Right Circular Cylinder	RCC	Vx	Vy	Vz	Hx	Hy	Hz	1 of 2
		R	-	-	-	-	-	2 of 2
Right Elliptic Cylinder	REC	Vx	Vy	Vz	Hx	Hy	Hz	1 of 2
		R1x	R1y	R1z	R2x	R2y	R2z	2 of 2
Ellipsoid of Revolution	ELL	V1x	V1y	V1z	V2x	V2y	V2z	1 of 2
		R	-	-	-	-	-	2 of 2
Truncated Cone	TRC	Vx	Vy	Vz	Hx	Hy	Hz	1 of 2
		R_1	R_2	-	-	-	-	2 of 2
Right Angle Wedge	RAW	Vx	Vy	Vz	H1x	H1y	H1z	1 of 2
		H2x	H2y	H2z	H3x	H3y	H3z	2 of 2
Arbitrary Polyhedron	ARB	V1x	V1y	V1z	V2x	V2y	V2z	1 of 5
		V3x	V3y	V3z	V4x	V4y	V4z	2 of 5
		V5x	V5y	V5z	V6x	V6y	V6z	3 of 5
		V7x	V7y	V7z	V8x	V8y	V8z	4 of 5
		Face Descriptions (See Note following page)						
Truncated Elliptical Cone	TEC	Vx	Vy	Vz	Hx	Hy	Hz	1 of 3
		Nx	Ny	Nz	Ax	Ay	Az	2 of 3
		R_1	R_2	P	-	-	-	3 of 3

Note: Each of the six faces of an ARB are described by a four-digit number giving the number of the four vertex points at the corners. The order of specification of the four points is completely arbitrary. The point specification format is 6(E10.3) starting in Column 11. An example is shown below.



FACE	1	2	3	4	5	6
PTS	1653.	3548.	4278.	1762.	1243.	5678.

Figure A.2.5 - Example of Arbitrary Polyhedron

When the number of faces is less than six, the remaining face description(s) must be zero, and must appear at the end of the list.

If a face has three vertices, the omitted position may be either 0 or a repeat of one of the other vertices.

Eight vertices must always be supplied. Those that do not appear in face descriptions are ignored.

2. Region Cards

Each region must be numbered and described by a logical combination of the bodies which make up that region. Use as many cards as necessary to describe each region and begin each region on a new card. The input format, described below, is (2x, A3, 5x,9 (A2, I5)).

Columns	Input
1-2	Blank
3-5	Arbitrary hollerith data
6-10	Blank
11-73	Divided into nine fields, of 7 columns each. The first two columns of each field are reserved for the OR operator. The third column is for the (+) or (-) operator. The last four columns are for the body number.

Use as many cards of the above type as needed to complete a region description, but leave Columns 1-10 blank on all continuation cards.

The last region description card must be followed by a card containing END in Columns 3, 4, and 5. This informs the code that all regions have been described.

APPENDIX B

ORGANIZATION OF THE MASTER-ASTER ARRAY

The first part of the MASTER-array contains the unperturbed cross section data in the same format as the output of SAM-X (processor of ENDF/B cross section data), the details of which are referred to in a separate report of processor SAM-X[1]. The remainder of the MASTER-array is described below.

The capitalized name in each box refers to a "pointer". These "pointers" are used to locate sections of data with a minimum of calculation.

	Contents	Comments
(1)	LSCORE Flux scores for each statistical aggregate	The scores are accumulated and stored by CARLO and FLUP. The scores are stored as a function of energy and scoring region.
(2)	LREGT Region-dependent parameters	This section of the array contains region-dependent parameters stored two computer words per region. The actual data are discussed in the UNPR section of this report. The data are read in and stored by INPUTD.
(3)	LNCOL Number of collisions per region	

	Contents	Comments
(4)	LBIRTH The number of births per region	
(5)	LDEATH The number of deaths per region	
(6)	LESCAP The number of escapes per region	
(7)	LNDEG The number of degrades per region	
(8)	LNABS The number of absorptions per region	

For items (3) through (8) the starting locations are computed in INPUTD. The counts are accumulated in CARLO and are printed by TALLY.

(9)	LRAW Region weights	The actual region weights to be used for region importance. The weights are read in by INPUTD.
(10)	LREW Region energy weight sets	The energy weight sets for importance sampling. This section exists if energy importance is used in the problem. The data are read in by INPUTD.

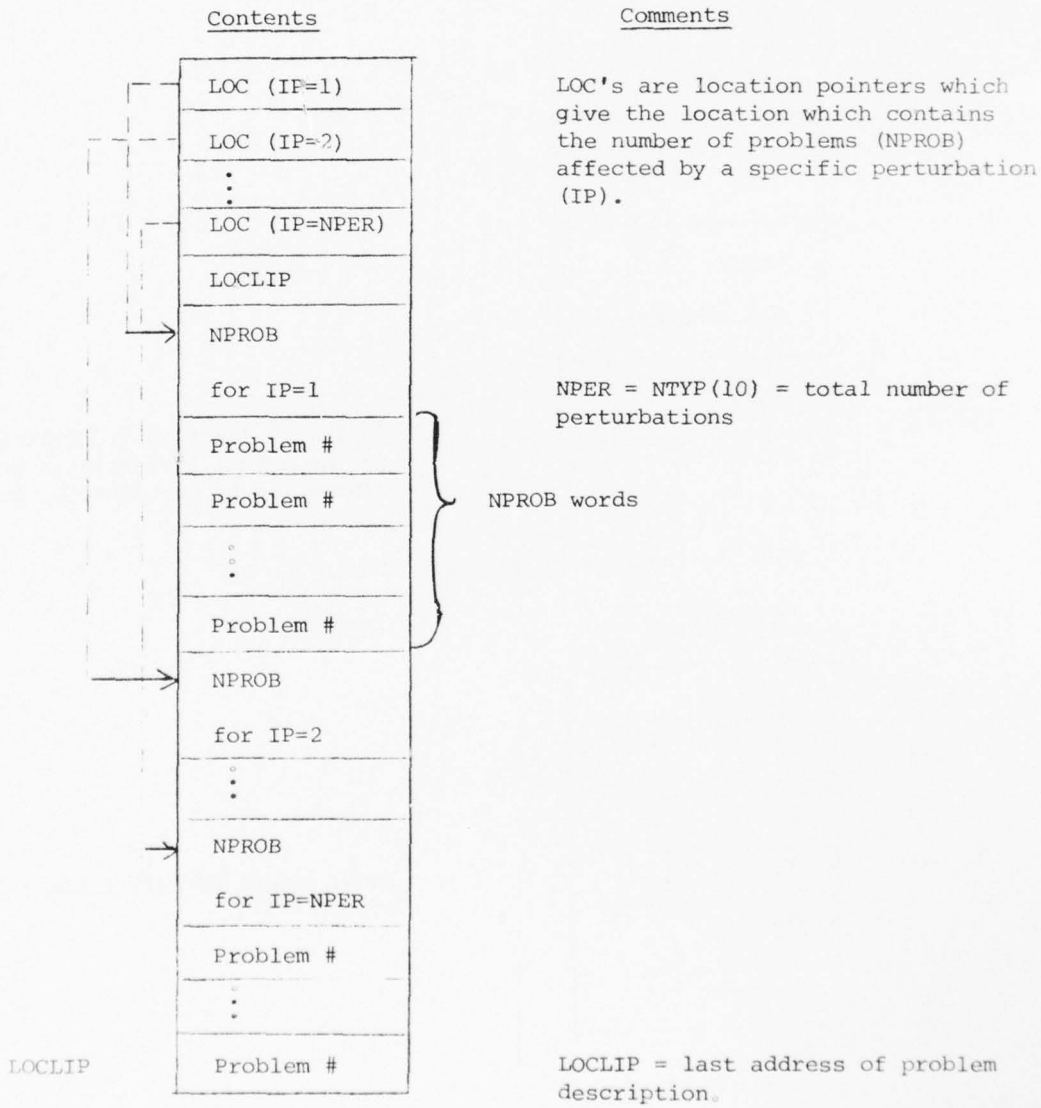
	Contents	Comments
(11)	LAIM Aiming Angles	The aiming angles for angular importance. Three words per angle denoting direction cosines are stored. The data are read by INPUTD. The array exists only if angular importance is used.
(12)	LAWS Region angular weight sets	The angular weight sets for angular importance. The array exists only if angular importance is used. The data are read by INPUTD.
(13)	KSOUR Source data	The energy, position, and direction data for the source distribution. The data are read in by SOUCAL.
(14)	LLAST Latent storage for supergroups	This section uses up all available room in the MASTER-array. Supergroup latents are stored here. Tapes will be used for latent storage if the available room is insufficient.

APPENDIX C

ORGANIZATION OF THE MISTER-SISTER ARRAY

The following sections describe the organization and contents of the MISTER-SISTER array in which all the perturbation data and necessary information about them reside.

C.1 - Storage Description for Problem Description



C.2 - Storage Description of Individual Perturbation Type

(All notations refer to text of Section 3.2)

	Contents	Comments
LOCLIP+1	LOCIP for IP=1	LOCIP's are location pointers which give the location where perturbation data of a specific perturbation (IP) begin.
	LOCIP for IP=2	
	⋮	
	LOCIP for IP=NPER	
LOCLIP+ NPER+1	BLANK	Following location (LOCLIP+NPER+1) is the actual perturbation data classified by perturbation types.

TYPE 1 - Composition (Present if NTYP(1)>0)

	Contents	Comments
LOCIP+0	ICOMP	
+1	NLM	
+2	EH	
+3	EL	these repeat NTYP(1)-1 times if NTYP(1)>1.
	C_1	
	C_2	
	⋮	
LOCIP+3 +NLM	C_{NLM}	

TYPE 2 - Whole Element Perturbation

	Contents	Comments
LOCIP+0	LOC(LOCELM)	LOC(LOCELM)=location of LOCELM in MASTER-array.
+1	LOC(LOCELP)	LOCELM=location where the unperturbed data of an element begin in MASTER-array.
+2	EH	
+3	EL	
+4	LOSAM for CHI-table	LOC(LOCELP)=location of LOCELP in MASTER-array.
+5	LOSAM for ENN-table	LOCELP=location where the perturbed element data begin in MASTER-array. (Only exists for perturbation type 2).
	Other perturbations of TYPE 2 repeat the above layout	LOSAM = location of sampling table.

TYPE 3, 4 and 5 - Total, Scattering or Inelastic Scattering Cross Section Perturbation

	Contents	Comments
LOCIP+0	LOC(LOCEJM)	
+1	NEP	
+2	EH	
+3	EL	
+4	FMULT	FMULT is significant only if NEP<2; LOCIP+5 to LOCIP+5+NEP exist only if NEP≥2
+5	LOCPS	
	$E_1 \geq EH$	
	E_2	
	E_3	
	⋮	
LOCIP+5+NEP	$E_{NEP} \leq EL$	

TYPE 3, 4 and 5 - continued

Contents	Comments
$\sigma(E_1)$	Cross section data at given energies
$\sigma(E_2)$	
⋮	
$\sigma(E_{NEP})$	
Other perturbations of TYPE 3 repeat the above layout	
Data for perturbations of TYPE 4	
Data for perturbations of TYPE 5	

TYPE 6 - Angular Distribution of Elastic Scattering

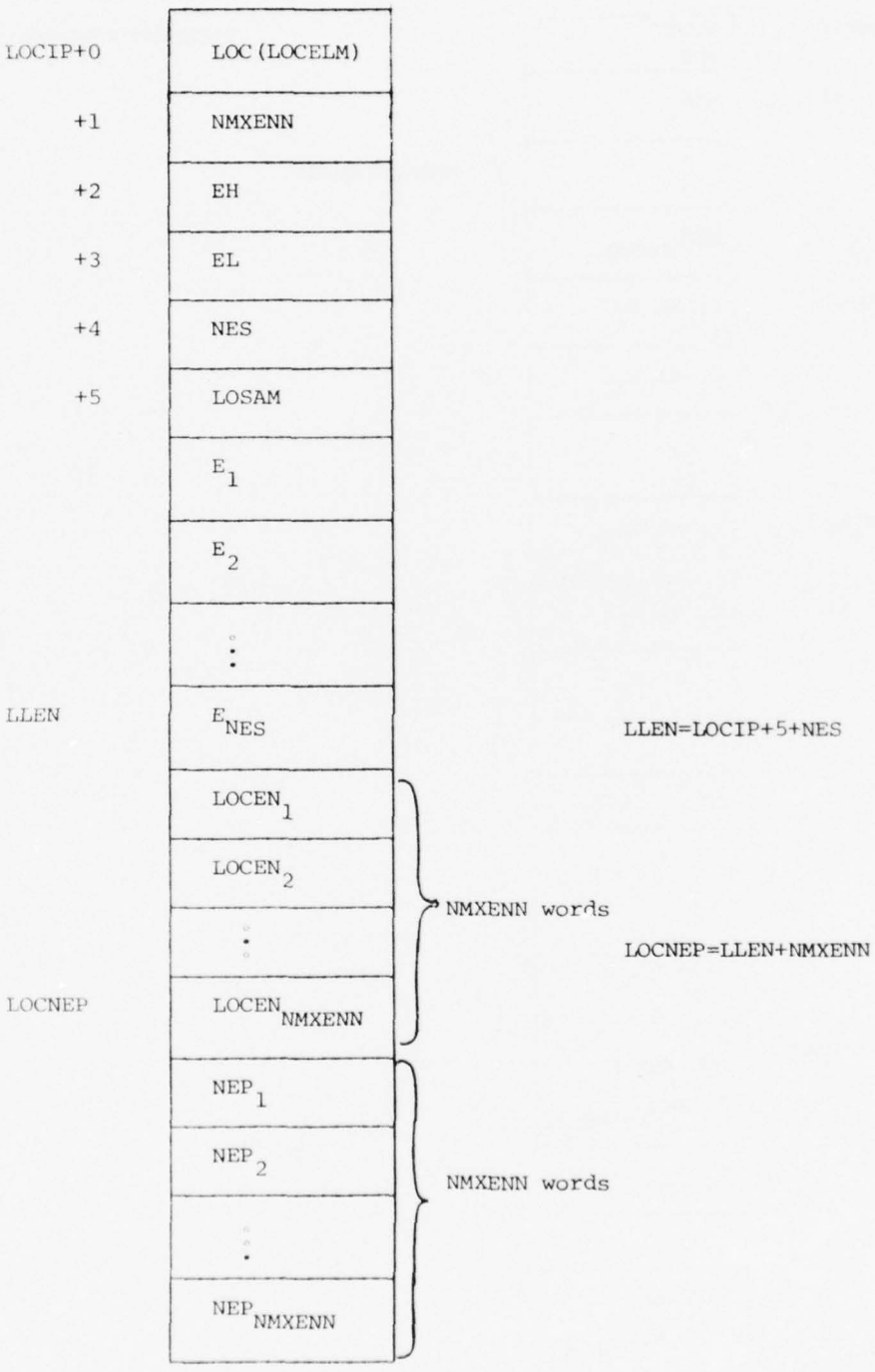
	Contents	Comments
LOCIP+0	LOC(LOCELM)	
+1	LOCNE	
+2	EH	
+3	EL	
+4	LOSAM	
+5	E_1	
	E_2	
	⋮	
	E_{NE}	
LOCNE+0	NE	LOCNE=LOCIP+5+NE
+1	BLANK	
+2	NMAXEK	
LOCEK+0	LCENEK	LOCEK=LOCNE+3
+1	$LOCEK_1$	
	$LOCEK_2$	NMAXEK words
	⋮	
	$LOCEK_{NMAXEK}$	

TYPE 6 - continued

	Contents	Comments
LOCNEK+0	NENEK =NE	LOCNEK=LOCEK+NMAXEK+1
+1	NEK_1	
	⋮	NMAXEK words
$LOCEK_1$+0	NEK_{NMAXEK}	
$LOCEK_1$+1	χ_1 at E_1	
	χ_1 at E_2	
	⋮	
$LOCEK_2$+0	χ_1 at E_{NEK_1}	
+1	χ_2 at E_1	
	χ_2 at E_2	
	⋮	
$LOCEK_3$+0	χ_2 at E_{NEK_2}	
	⋮	
$LOCEK_{NMAXEK}$+0	$\chi_{NMAXEK-1}$ at $E_{NEK_{NMAXEK-1}}$	
+1	χ_{NMAXEK} at E_1	
	⋮	
	χ_{NMAXEK} at $E_{NEK_{NMAXEK}}$	

Other perturbations of Type 6 repeat the above layout

TYPE 7 - Energy Distribution in Inelastic Continuum Scattering



TYPE 7 - continued

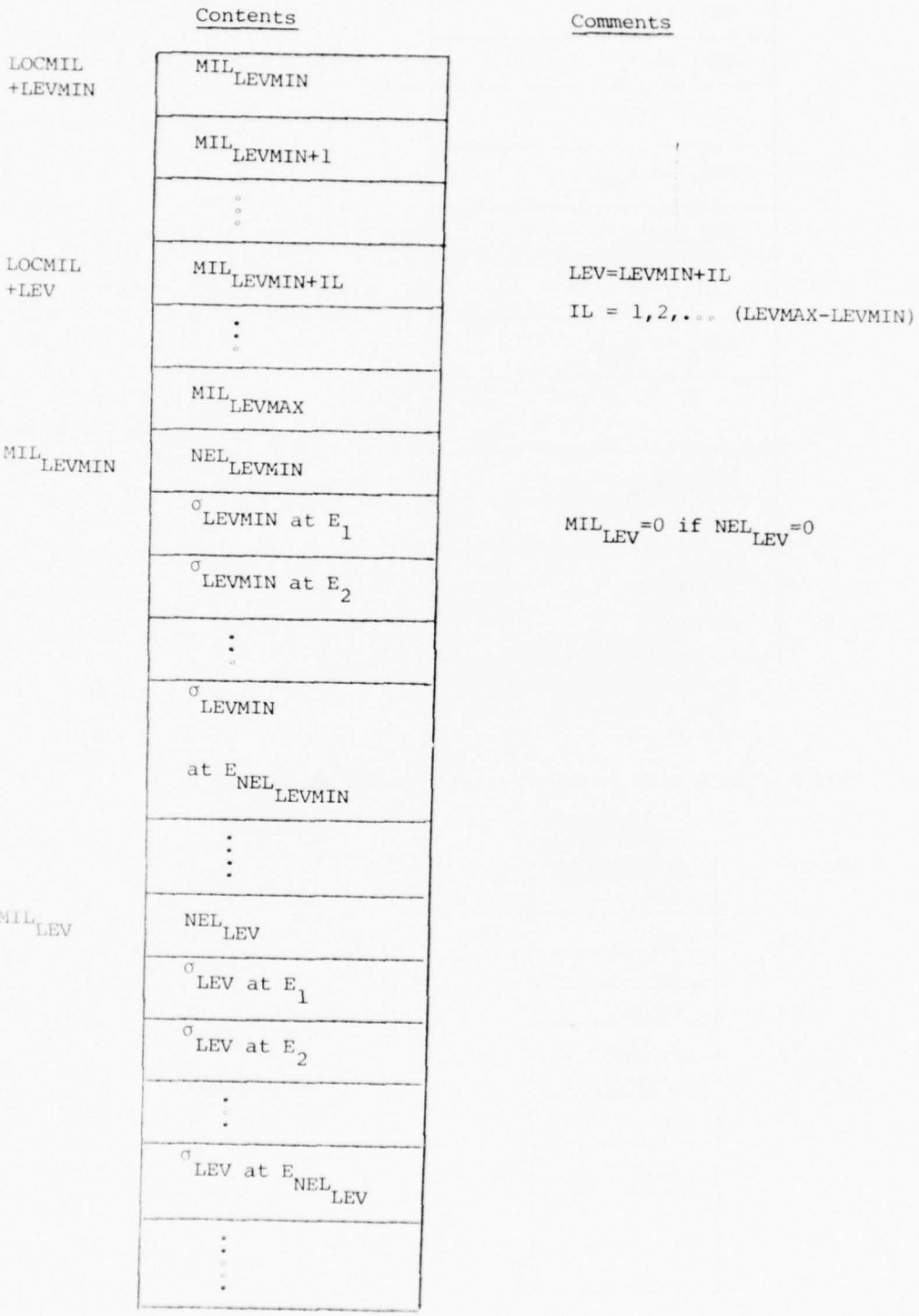
Contents	Comments
ENN_1 at E_1	
ENN_1 at E_2	
⋮	
ENN_1 at E_{NEP_1}	
ENN_2 at E_1	
⋮	
ENN_2 at E_{NEP_2}	
⋮	
ENN_{NMXENN} at E_1	
⋮	
ENN_{NMXENN} at $E_{NEP_{NMXENN}}$	

Other perturbations of TYPE 7 repeat the above layout

TYPE 8 - Cross Section for Inelastic Level Excitation

	Contents	Comments
LOCIP+0	LOC(LOCELM)	
+1	NES	
+2	EH	
+3	EL	
+4	LEVMIN	
+5	LEVMAX	
LOCE	LOCMIL	LOCE=LOCIP+6
	E_1	
	E_2	
	⋮	
	E_{NES}	

TYPE 8 - continued



TYPE 8 - continued

Contents	Comments
NEL_{LEVMAX}	
σ_{LEVMAX} at E_1	
σ_{LEVMAX} at E_2	
⋮	
σ_{LEVMAX} at $E_{NEL_{LEVMAX}}$	

Other perturbations of TYPE 8 repeat the above layout

TYPE 9 - Angular Distribution of Discrete Inelastic Scattering

	Contents	Comments
LOCIP+0	LOC(LOCELM)	
+1	NENS	
+2	EH	
+3	EL	
+4	LEVMIN	
+5	LEVMAX	
+6	LOCMIL	
+7	E_1	
	E_2	
	⋮	
	E_{NENS}	
LOCMIL +LEVMIN	MIL_{LEVMIN}	
	$MIL_{LEVMIN+1}$	
	⋮	

TYPE 9 - continued

	Contents	Comments
LOCMIL+LEV	$MIL_{LEVMIN+IL}$	LEV=LEVMIN+IL IL= 1,2,...(LEVMAX-LEVMIN)
	⋮	
	MIL_{LEVMAX}	
MIL_{LEVMIN}	NEL_{LEVMIN}	
	LOCNMU for E_1	
	LOCNMU for E_2	
	⋮	
	LOCNMU for $E_{NEL_{LEVMIN}}$	
	NMU at E_1	
	μ_1=FMU_1=-1.0	
	μ_2=FMU_2	
	⋮	*NMU words at E_1*
	μ_{NMU}=FMU_{NMU}=1.0	
	PP=dP/dμ at μ=-1.0	
	⋮	
	PP at μ=+1.0	
	NMU at E_2	
	μ_1	
	μ_2	
	⋮	NMU words at E_2
	μ_{NMU}	

TYPE 9 - continued

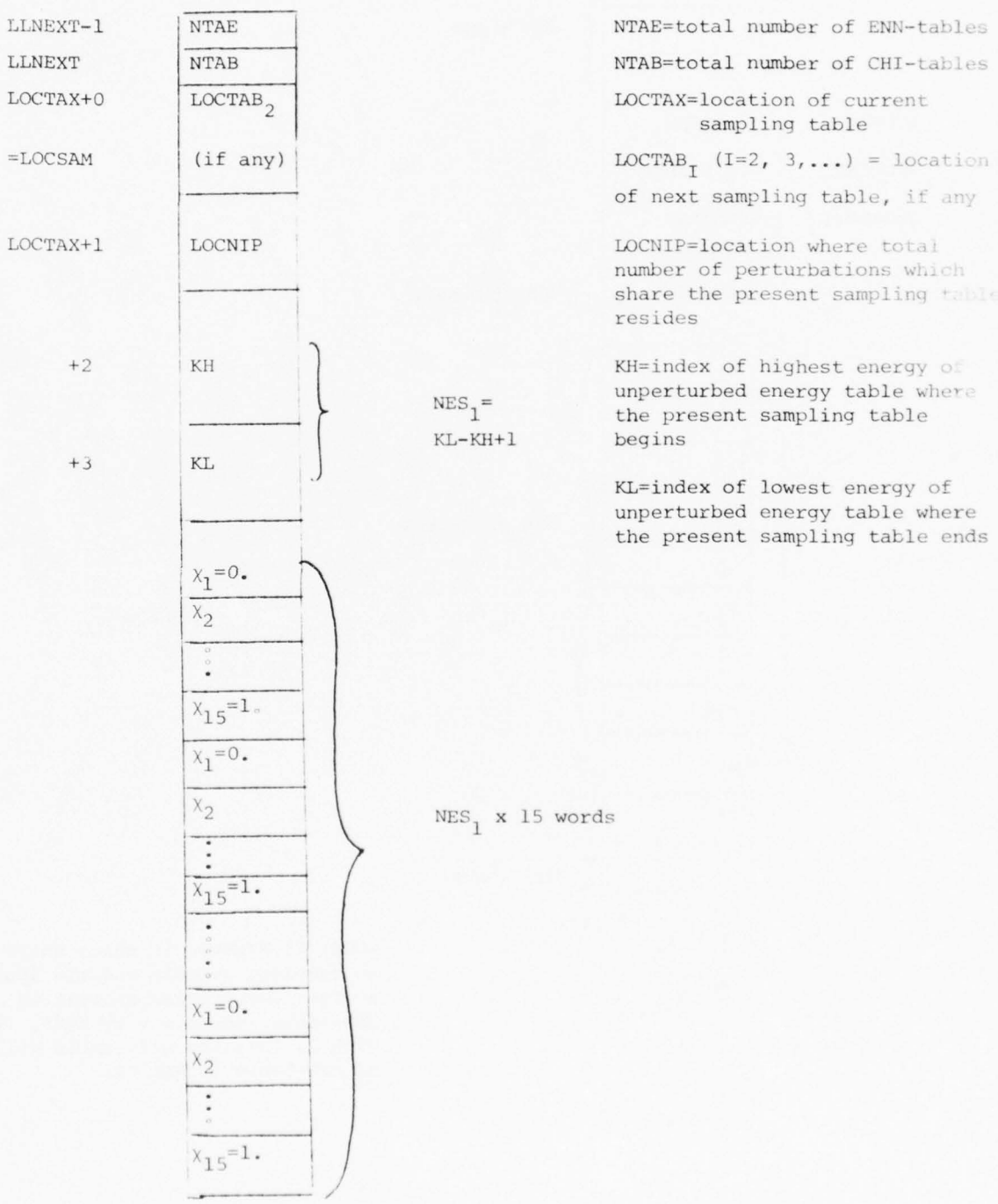
	Contents	Comments
	PP at μ=-1.0	NMU words at E_2
	⋮	
	PP at μ=+1.0	
	⋮	
	NMU at E_{NES}	
	μ_1 at E_{NES}	
	⋮	
	μ_{NMU} at E_{NES}	
	PP at μ=-1.0	
	⋮	
	PP at μ=+1.0	
$MIL_{LEVMIN+1}$	$NEL_{LEVMIN+1}$	
	LOCNMU for E_1	
	LOCNMU for E_2	
	⋮	
	LOCNMU for $E_{NEL_{LEVMIN+1}}$	
	NMU at E_1	
	μ_1 at E_1	
	⋮	
	μ_{NMU} at E_1	
	PP	
	⋮	
	etc.	

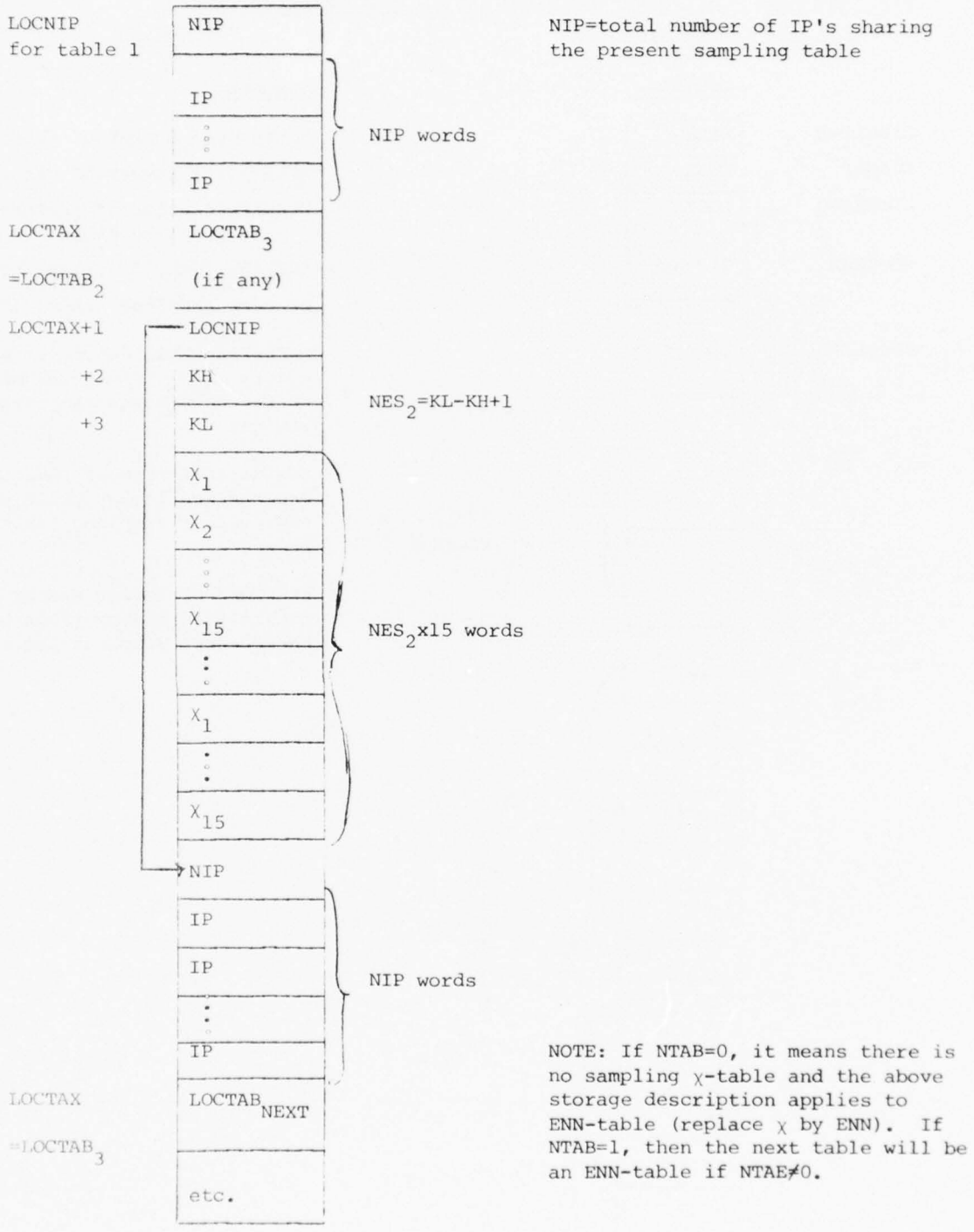
Other perturbations of TYPE 9 repeat the above layout

TYPE 10 - Source Spectrum

	Contents	Comments
LOCIP+0	NES	
+1	BLANK	
+2	EH>EHIGH	
+3	EL<ELOW	
+4	E_1	
	E_2	
	⋮	
LOCIP+3+NES	E_{NES}	
	$(\Delta S/\Delta E)_1$	
	$(\Delta S/\Delta E)_2$	
	⋮	
	$(\Delta S/\Delta E)_{NES}$ (ignore this last one)	
	Other perturbations of TYPE 10 repeat the above format	End of perturbation data
	BLANK	
LLNEXT	BLANK	Starting from location (LLNEXT-1) storage available for next perturbation data (e.g., sampling CHI- or ENN-tables)

C.3 - Storage Description for Sampling CHI- and ENN-tables of One Energy Band

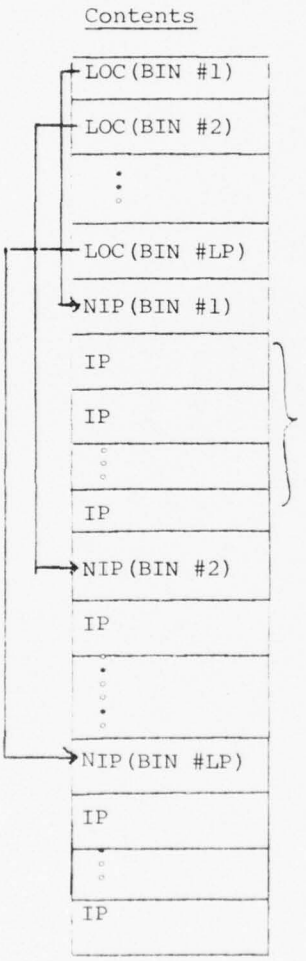



Contents
Comments
LOCNIP
for table 1
NIP
NIP=total number of IP's sharing the present sampling table
IP
IP
NIP words
LOCTAX
LOCTAB3
=LOCTAB2
(if any)
LOCTAX+1
LOCNIP
+2
KH
+3
KL
NES2=KL-KH+1
χ1
χ2
χ15
NES2x15 words
χ1
χ15
NIP
IP
IP
NIP words
IP
LOCTAX
LOCTABNEXT
=LOCTAB3
etc.
NOTE: If NTAB=0, it means there is no sampling χ-table and the above storage description applies to ENN-table (replace χ by ENN). If NTAB=1, then the next table will be an ENN-table if NTAE≠0.

APPENDIX D

ORGANIZATION OF THE IPBIN-ARRAY

The following section describes the organization and contents of the IPBIN-array.



NIP words for BIN #1

Comments

LOC's are pointers which give the location which contains the total number of perturbations (IP's) affecting a given energy bin in PETAB-array (cf. Section 2.2). LP = total number of energy bins in PETAB-array.

APPENDIX E

BOUNDED FLUX-AT-A-POINT (BFAP) ESTIMATION

E.1 Introduction

In many instances, the availability of a point estimation capability represents a desirable extension of the ordinary track length or volume estimation method. However, unless special biasing procedures are employed, flux-at-a-point estimation effects infinite variance.

A very efficient scheme, developed by Steinberg and Kalos[3], involves biased selection of source and collision points such that, not only are subsequent "last flight" estimates at point detectors made with finite variance, but, in addition, all estimates are made with a finite upper bound. This combination of biased selection and "last flight" estimation, the so-called bounded flux-at-a-point (BFAP) estimation, is superior to the so-called "once-more-collided" flux-at-a-point (FAP) estimation[1], because fewer histories are required to achieve a given statistical accuracy.

The sections which follow describe the mathematical basis for, and the coding implementation of the algorithms comprising the BFAP estimation procedure.

E.2 Theory

E.2.1. Point Estimation

The following procedure can be used to make flux-at-a-point estimates. In the course of each Monte Carlo history, at the time of position (source or collision) selection, a virtual ray is traced from the selected position to the detector. The estimator term, f, is given by the expression (where $\bar{\Omega}$ is the direction vector of the virtual ray):

$$f = Wg(\bar{\Omega})\exp(-\int\sigma(s)ds)/4\pi R^2$$

where W is the particle weight at the selected position, $g(\bar{\Omega})$ is the differential directional distribution (discussed below), σ is the total macroscopic cross-section, and R is the distance between the selected position and the detector. The integration in the exponential is along the straight line path from the selected position to the detector.

The term $g(\bar{\Omega})$ out of a source would be constant for isotropic distributions; otherwise it is a prescribed function of direction. At a collision, the situation is more complicated. The collision procedure is usually carried out in several selection steps: (1) position, (2) target element, (3) reaction process, (4) scattering angle. The most efficient place to carry out the point estimation is between steps (3) and (4), where W reflects the state of the particle after step (3). $g(\bar{\Omega})$ is then, simply, the (laboratory) angular distribution of the selected reaction for the selected target, and is actually a function of $\bar{\Omega}_o \cdot \bar{\Omega}$, where $\bar{\Omega}_o$ is the particle direction entering collision.

The principal problem associated with such an estimation procedure is the presence of the R^2 term in the denominator of f. If the selected position is near the detector, the estimator is arbitrarily large in value. As a means of overcoming this problem, Steinberg and Kalos[3] devised a procedure (discussed below) where the position selection is biased so that W contains a compensating factor proportional to R^2. This then leads to an upper bound for f.

E.2.2. Bounded Estimation

Since a full discussion of the theory of bounded estimation for point detectors is given in Reference 3, only the essentials will be described. Consider a region around the detector at x_D (e.g., a sphere of radius R_o centered at the detector, or a region of some other shape containing such a sphere). Then, if the position selection is biased to be uniform in the distance from the detector, the compensating weight factor contains a term proportional to R^2, where R is the distance between the detector and the selected position.

When the selected position x is a collision position, care must be taken that the distance to the previous particle position x_o is also biased properly to avoid a singularity of the form R_1^{-2}, where R_1 is the distance between the previous position and the collision position. This can be accomplished by first biasing the direction out of the previous collision so that selection of the angle α between $(x-x_o)$ and (x_D-x_o) is proportional to α rather than the "natural" $\cos\alpha$ (ignoring local anisotropy). Then the position along the path is selected from a probability density with a factor $1/R^2$.

In Reference 3, an implementation using a reselection procedure was described, where x is reselected within the detector region by reselecting and the distance along the ray. (If the selected position is a source position, the problem does not exist, and the method described in Reference 3 applies.)

The principal drawback of this procedure is the need for the availability of the angular distribution data to get the proper weight adjustment for the selection. If the previous position was also a collision, this angular distribution data is a function of the particle energy before the previous collision, which might not be available at the time the reselection takes place, because a different band of cross section data is in the machine. To avoid this programming difficulty, the angle portion of the biasing is carried out concurrently with the selection of the direction out of the previous position. The biasing of the distance along the ray is carried out later in the course of selecting the collision position.

E.2.3. Multiple Detectors

In general, the procedures described above can be easily implemented when there are several point detectors. The estimation procedure becomes, essentially, a repetition of the single detector scheme, with the added complication of possible interactions between the detectors. The algorithms utilized to resolve this multi-detector complication are discussed in Appendix F.

E.3 Code Implementation

The implementation of BFAP estimation comprises several distinct aspects: (1) problem initialization; (2) angle reselection; (3) position selection; and (4) resolution of multiple detector conflicts. The first three aspects are discussed in the sections that follow. Multiple detector effects are the subject of Appendix F.

E.3.1. Problem Initialization

After reading in user supplied information about the point detectors, two basic characteristics are precomputed for each detector. The first characteristic is the so-called "critical radius", which defines a sphere of influence about the detector point, also referred to as the "critical sphere". The algorithm for computing* this radius is

$$R_k = (\bar{\mu}_k)^{-1} \qquad \text{(E-1)}$$

where $\bar{\mu}_k$ is the total macroscopic cross section of the material region designated for the k-th detector, evaluated for a nominal microscopic cross section of 1 barn/atom.

The second characteristic determined for each detector is a "critical sphere overlap" flag, which is utilized in the resolution of multiple detector conflicts. If $\{\bar{x}_k\}$ are the detector locations, then the algorithm for determining these overlap flags $\{L_k\}$ (initialized to 0) is

$$|\bar{x}_k - \bar{x}_i|^2 < (R_k + R_i)^2,\ i \neq k;\ \text{set } L_k = 1. \qquad \text{(E-2)}$$

---

* The user may, optionally, supply a value for the critical radius directly, as described in the section on point detector input.

E.3.2 Angle Reselection

Angle reselection is indicated whenever an originally selected (OS) ray intersects the critical sphere of a live detector. In addition, for post scattering (as opposed to source) directions, the corresponding post scattering energy must be recomputed. Furthermore, for near threshold inelastic or hydrogen scattering of neutrons, for which the effective mass of recoiling nucleus is $A' \leq 1$ [neutron mass], a special treatment is required, since a range of scattered directions becomes physically impossible.

E.3.2.1. Angle Reselection (General)

Let $\bar{W}$ be the originally selected (OS) direction. The algorithm for determining the intersection of live critical spheres proceeds as follows: For each live detector, let $\bar{W}_k = (\bar{x}_k - \bar{x})/|\bar{x}_k - \bar{x}|$, where $\bar{x}_k$ is the position of the k-th detector, and $\bar{x}$ is the particle position. Let $\delta_k = \bar{W} \cdot \bar{W}_k$. Then, if

$$\delta_k^2 > 1 - R_k^2/|\bar{x} - \bar{x}_k|^2, \quad (\delta_k > 0) \tag{E-3}$$

the k-th critical sphere is intersected by the OS ray. If no live detector satisfies the conditions of (E-3), no reselection is necessary, and the remaining procedure is bypassed. If more than one live detector sphere is intersected by the OS ray, a "multiple detector conflict" (MDC) exists. Even if only one detector sphere is intersected, an MDC may have to be resolved due to sphere or cone overlap (see Appendix F).

Ultimately, subsequent to possible resolution of an original MDC, at most one live detector sphere, k, will be intersected by the OS ray. The angle reselection, then, proceeds as follows: choose an angle θ^* uniformly in the range $[\theta_H, \theta_L]$ given by

$$r = \min \{R_k/|\bar{x} - \bar{x}_k|, 1.0\} \tag{E-4a}$$

$$\theta_H = \sin^{-1}(r) \tag{E-4b}$$

$$\theta_L = -\theta_H \tag{E-4c}$$

For near threshold inelastic or hydrogen scattering, the algorithm of (E-4) is replaced by the special procedure described in the next section.

The reselected angle θ^* yields a reselected (RS) direction (or ray) $\bar{W}^*$ given by

$$\bar{W}^* = \alpha\bar{W} + \beta\bar{W}_k \qquad \text{(E-5a)}$$

where

$$\alpha = \sin\theta^*/\sin\theta \qquad \text{(E-5b)}$$

$$\beta = \sin(\theta-\theta^*)/\sin\theta \qquad \text{(E-5c)}$$

$$\theta = \cos^{-1}(\bar{W}\cdot\bar{W}_k) \qquad \text{(E-5d)}$$

To avoid the singularity when $\theta=0$, the following algorithm precedes (E-5): Let $\bar{W} = \bar{W}_k = (v_1, v_2, v_3)$. Find i for which $|v_i|$ is smallest. Let new $\bar{W}$ be the vector formed by adding 0.01 to the i-th component of $\bar{W}_k$, and normalizing to unity.

Finally, the particle weight must be adjusted by a factor

$$W_a = C\, q(\Delta^*)/q(\Delta) \qquad \text{(E-6a)}$$

where q is the sampling density for lab angle cosines (Δ and Δ^* are the OS and RS values, respectively), and

$$C = |\sin\theta^*|\,(\theta_H - \theta_L)/I(\theta_H,\theta_L) \qquad \text{(E-6b)}$$

$$I(\theta_H,\theta_L) = \cos\theta_L - \cos\theta_H,\ \theta_L \geq 0$$

$$= 2 - \cos\theta_H - \cos\theta_L,\ \theta_L < 0 \qquad \text{(E-6c)}$$

E.3.2.2 Special Procedure For $A' \leq 1$ Case

For near threshold inelastic and hydrogen scattering, where the (effective) weight of the recoiling nucleus $A' \leq 1$, the general algorithms (E-3) and (E-4) are modified as follows: in addition to the constraint of (E-3), the condition

$$\bar{W}\cdot\bar{W}_k < \bar{W}_o\cdot\bar{W}_k \qquad \text{(E-7)}$$

effects a bypass of angular reselection, where $\bar{W}_o$, $\bar{W}$, and $\bar{W}_k$ are the pre-scattering, OS, and the direction to the k-th detector, respectively.

If (E-7) is not satisfied, the special procedure for $A' \leq 1$ proceeds with the computation of three angles, β, δ, γ in the range $(0, \pi)$.

$$\beta = \sin^{-1}(A'); \qquad 0 \leq \beta \leq \pi/2 \tag{E-7a}$$

$$\delta = \cos^{-1}(\bar{W}_k \cdot \bar{W}_o) \tag{E-7b}$$

$$\gamma = \min(\delta, \theta_H) \tag{E-7c}$$

where θ_H is given by (E-4b).

If $\beta \geq \gamma + \delta$, the remainder of the special procedure is bypassed. Otherwise, define $\psi_M = \frac{\pi}{2}$, $(\beta > \delta)$;

$$= \cos^{-1}\left[(\cos\beta - \cos\delta\cos\gamma)/(\sin\delta\sin\gamma)\right] \quad (\beta \leq \delta) \tag{E-8}$$

Choose ψ uniformly in $\left[0, \psi_M\right]$. Compute a temporary $\bar{W}$, as input to the reselection, using

$$\bar{W} = A\,\bar{W}_k + B\,\bar{W}_o + C\,(\bar{W}_k \times \bar{W}_o) \tag{E-9}$$

where

$$A = \cos\delta(1 - \cos\psi) \tag{E-10a}$$

$$B = \cos\psi \tag{E-10b}$$

$$C = \pm \sin\psi \tag{E-10c}$$

The sign of C is chosen at random with equal probability.

As a final preparation to the reselection procedure, it is necessary to define θ_H, θ_L, and θ. Substituting (E-9) into (E-5d) yields $\theta = \delta$.

Let $U = \cos\psi\sin\delta$ (E-11a)

$$V = \sqrt{\sin^2\beta - \sin^2\psi\sin^2\delta} \tag{E-11b}$$

$$X = \cos^2\psi\sin^2\delta + \cos^2\delta \tag{E-11c}$$

Define $\theta_{\pm}$ in the range $(0,2\pi)$ using:

$$\cos\theta_{\pm} = (\cos\beta\cos\delta \pm UV)/X; \quad \psi < \pi/2 \tag{E-12a}$$

$$\sin\theta_{\pm} = \frac{\cos\beta - \cos\delta\cos\theta_{\pm}}{\sin\delta\cos\psi}; \quad \psi < \pi/2 \tag{E-12b}$$

$$\cos\theta_{\pm} = \cos\beta/\cos\delta \; ; \; \psi = \pi/2 \tag{E-12c}$$

$$\sin\theta_{\pm} = \pm\sqrt{1 - \cos^2\theta_{\pm}} \; ; \; \psi = \pi/2 \tag{E-12d}$$

Then, using $\theta_{\pm}$ as defined above:

$$\theta_1 = \max(\theta_+,\theta_-) \; ; \quad \beta \leq \delta \tag{E-13a}$$

$$\theta_2 = \min(\theta_+,\theta_-) \; ; \quad \beta \leq \delta \tag{E-13b}$$

$$\theta_1 = \min(\theta_+,\theta_-) \; ; \quad \beta > \delta \tag{E-13c}$$

$$\theta_2 = \max(\theta_+,\theta_-) - 2\pi \; ; \quad \beta > \delta \tag{E-13d}$$

$$\theta_H = \min(\theta_1,\gamma) \tag{E-13e}$$

$$\theta_L = \max(\theta_2,-\gamma) \tag{E-13f}$$

An additional weight adjustment factor C must be computed by:

$$C = \frac{\psi_M I(\theta_H,\theta_L)}{\pi - \Omega - \eta\cos\beta - \psi_M\cos\gamma}$$

where $I(\theta_H,\theta_L)$ is given by (E-6c). Ω and η are angles between 0 and π, given by:

$$\eta = \cos^{-1}((\cos\gamma - \cos\beta\cos\delta)/\sin\beta\sin\delta) \tag{E-14a}$$

$$\Omega = \cos^{-1}((\cos\delta - \cos\beta\cos\gamma)/\sin\beta\sin\gamma) \tag{E-14b}$$

E.3.3. Position Selection

By means of the algorithms (discussed in Appendix F) designed to resolve an MDC, it is possible for a particle ray to intersect at most one sphere of radius R, centered at a live detector. If a critical sphere is not intersected, the probability density for position selection is given by $f_o(S)$ for "ordinary" tracking, viz.

$$f(S) = f_o(S) = \max_i \mu_i F_i \exp(-\mu_i S) \qquad \text{(E-15)}$$

where i is the problem index and

μ_i = attenuation coefficient (for problem i);

F_i = problem dependent weight;

S = geometric distance along the ray.

In practice, the track interval is subdivided into pieces, with break points defined at points where the index corresponding to the maximum (as computed in E-15 above) changes.

If a live critical sphere of radius R is intersected, the probability density f(S) is determined as follows. Let $f_o(S)$ be defined as in (E-15), and consider a subinterval over which one particular index i defines the maximum used to obtain $f_o(S)$. Then f(S) assumes one of two forms, viz.

$$f(S) = Cf_o(S) \qquad \text{(E-16a)}$$

$$f(S) = R^2 f_o(S_A)/h(S) \qquad \text{(E-16b)}$$

where the following algorithms determine the specific form for f(S).

Let S_A and S_B $(>S_A)$ be the end points of the subinterval and let

$$h(S) = R_o^2 + (S-S_o)^2 \qquad \text{(E-16c)}$$

where

R_o = distance between ray and detector;

S_o = distance along ray to the point at which R_o is the distance to the detector.

Noting that the procedure is operative only when $R_o < R$, three breakpoints are defined initially (see Figure E-1):

$$B_1 \equiv S_L = S_o - \sqrt{R_o R - R_o^2} \qquad \text{(E-17a)}$$

$$B_2 \equiv S_o \qquad \text{(E-17b)}$$

$$B_3 \equiv S_H = S_o + \sqrt{R^2 - R_o^2} \qquad \text{(E-17c)}$$

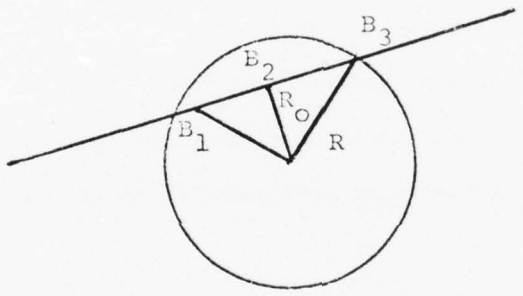


Figure E.1 - Breakpoint Definitions

If a breakpoint falls between S_A and S_B, the interval is divided at the breakpoint.

Case 1: $S < S_L$

In this case the appropriate form for f(S) is given by (E-16a), with C given by R/R_o, viz.

$$f(S) = Rf_o(S)/R_o. \tag{E-18}$$

Case 2: $S_L<S<S_o$

Compute $r=h(S_B)/h(S_A)$.

For $r>1/2$

$$f(S) = R^2 f_o(S)/h(S_B). \tag{E-19}$$

Otherwise, for $r<1/2$, further tests are necessary. If $\mu_i(S_B-S_A)<\ln 2$, then (E-16b) is used. If the latter test fails, a new breakpoint S_B is computed, viz.

$$S_B = \max\ (S_\alpha, S_\beta) \tag{E-20a}$$

where S_α and S_β satisfy

$$h(S_\alpha)/h(S_A) = 1/2 \tag{E-20b}$$

$$\mu_i(S_\beta-S_A) = \ln 2. \tag{E-20c}$$

Then f(S) is given by (E-19) if $S_\beta = S_\alpha$; and (E-16b) applies for $S_B = S_\beta$.

Case 3: $S_o < S<S_H$

The algorithms of Case 2 apply, with

$$r = h(S_A)/h(S_B) \tag{E-21a}$$

$$C = R^2/h(S_A) \tag{E-21b}$$

and S_α defined by

$$h(S_A)/h(S_\alpha) = 0.5. \tag{E-21c}$$

When $S>S_H$, f(S) reverts to the ordinary tracking density, $f_o(S)$. In all cases, the particle weight adjustment is given by

$$W_i = \mu_i \exp(-\mu_i S)/f(S) \tag{E-22}$$

where i is the problem index.

APPENDIX F

MULTIPLE DETECTOR CONFLICTS (MDC)

F.1 Introduction

Since the special biasing schemes of the BFAP estimation procedure are based on the concept of detector spheres of influence, the simultaneous presence of several detectors defines potentially overlapping regions of influence. Such regions represent multiple detector conflicts (MDC). The MDC are resolved via the "live detector" concept described in the sections that follow.

F.2 The MDC Condition

Relevant to the aspect of angle reselection, the MDC condition exists whenever any pair of live detectors satisfies the "cone overlap test" (COT). Let $\bar{X}$, $\bar{X}_k$, and $\bar{X}_\ell$, be the positions of the particle, and the k-th, and the ℓ-th detector, respectively. Let $\beta_{k\ell} = \bar{W}_k \cdot \bar{W}_\ell$, where $\bar{W}_k = (\bar{X}_k - \bar{X})/|\bar{X}_k - \bar{X}|$, and $\bar{W}_\ell$ is similarly defined. Then, if

$$\beta_{k\ell} \geq \sqrt{\left(1 - \frac{R_k^2}{|\bar{X}-\bar{X}_k|^2}\right)\left(1 - \frac{R_\ell^2}{|\bar{X}-\bar{X}_\ell|^2}\right)} \qquad - \frac{R_k R_\ell}{|\bar{X}-\bar{X}_k||\bar{X}-\bar{X}_\ell|}$$

the COT is satisfied, and an MDC exists.

Although references to "sphere overlaps" (see algorithm (E-2)) and "multiple intersections" (see algorithm (E-3)) also imply the existence of an "angle" MDC, these tests comprise a sub-set of the COT. Finally, only a sphere overlap is a significant MDC for position reselection.

F.3 Resolution of an MDC

An MDC may be resolved by Russian roulette, in which one live detector is chosen for sampling purposes. The implication of this deactivation depends on the particular stage of the particle history at which it occurs.

F.3.1 Position Checking (Source)

After the selection of a source position at the start of a history, the resolution of an MDC is recorded by the appropriate setting of the live detector "position flag", KDLIV. The relevent algorithms are best summarized by a logical flow chart:

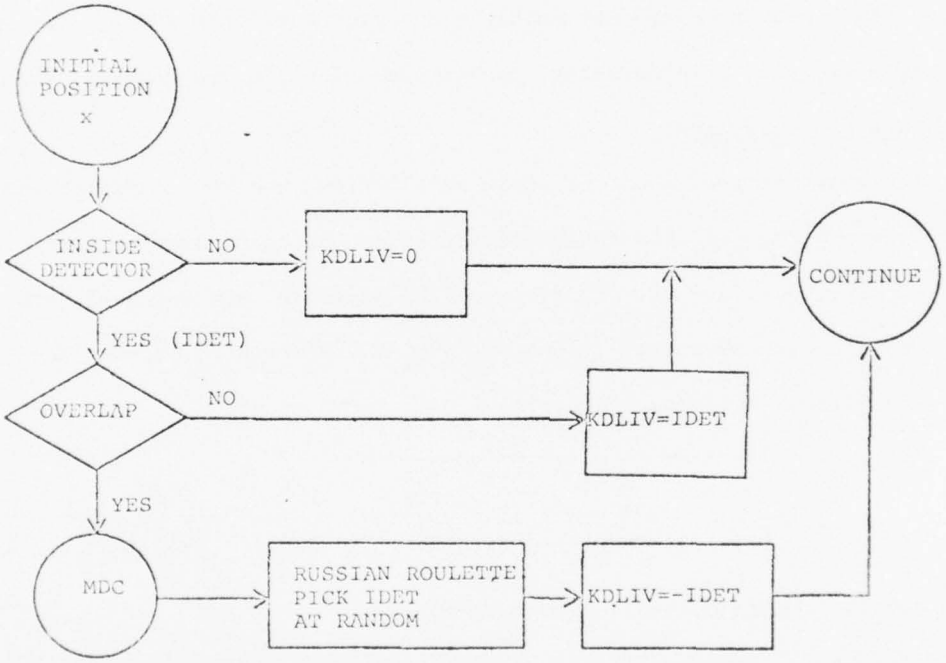


FIGURE F-1

Source Position Checking Algorithms

F.3.2 Direction Checking

Subsequent to position checking (both at a source and a collision* point), there are a series of direction checks aimed at resolving an angle MDC by appropriate setting of a live detector "direction flag", NDLIV. In order to distinguish between a latent and the current ray being tracked, another "direction flag", IDLIV assumes the role and the value of (the computed) NDLIV, whenever a source particle or latent is picked up for tracking.

As in the setting of KDLIV, the relevant algorithms for computing NDLIV are best summarized by a logical flow chart:

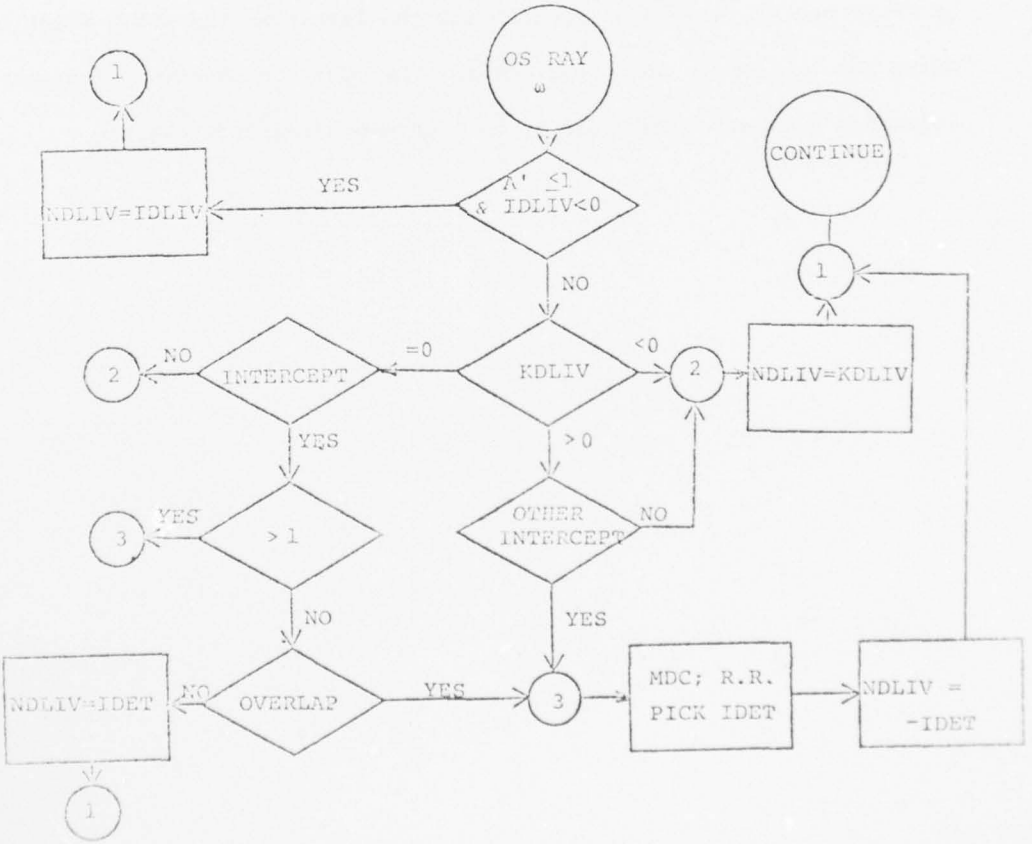


FIGURE F-2

Direction Checking Algorithms

*Refer to Section F.3.3

AD-A036 469 MATHEMATICAL APPLICATIONS GROUP INC ELMSFORD N Y F/G 18/11
SAMCEP: A CORRELATED MONTE CARLO NEUTRON AND GAMMA RADIATION TR--ETC(U)
FEB 77 H LICHTENSTEIN, H STEINBERG, J BROOKS DAAD05-75-C-0735
UNCLASSIFIED BRL-CR-330 NL

3 OF 3
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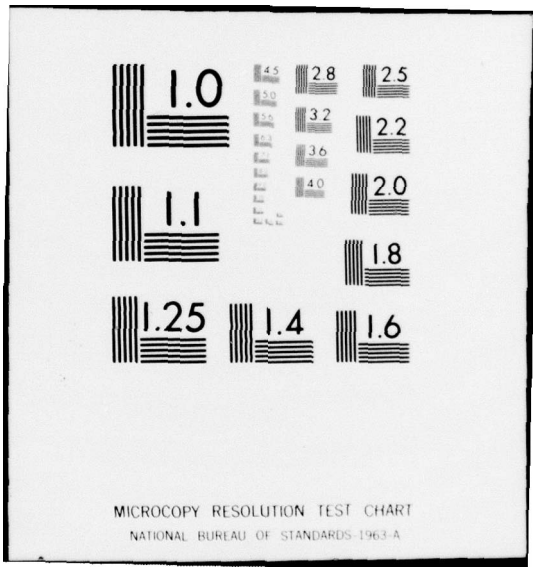
1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
4.5
5.0
MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

By means of the IDLIV (NDLIV) definition, sampling along the particle ray can be affected by at most one sphere, of radius R_k centered at a detector. Thus, for IDLIV>0, detector sphere #IDLIV is used; for IDLIV<0, # - IDLIV is used for sampling and a special weight adjustment is made (see Section F.3.4).

The value of IDLIV also influences the position checking at a collision point, as described in the next section.

F.3.3 Position Checking (Collision)

Subsequent to the selection of a collision point along the current ray, which is characterized by IDLIV (as opposed to NDLIV, which is computed for a latent), a value of KDLIV is computed for the latent to be stored. This value of KDLIV has the same significance for the latent as the KDLIV which is computed for the source position. Again, the position checking algorithms at the collision are best summarized by the corresponding flow chart:

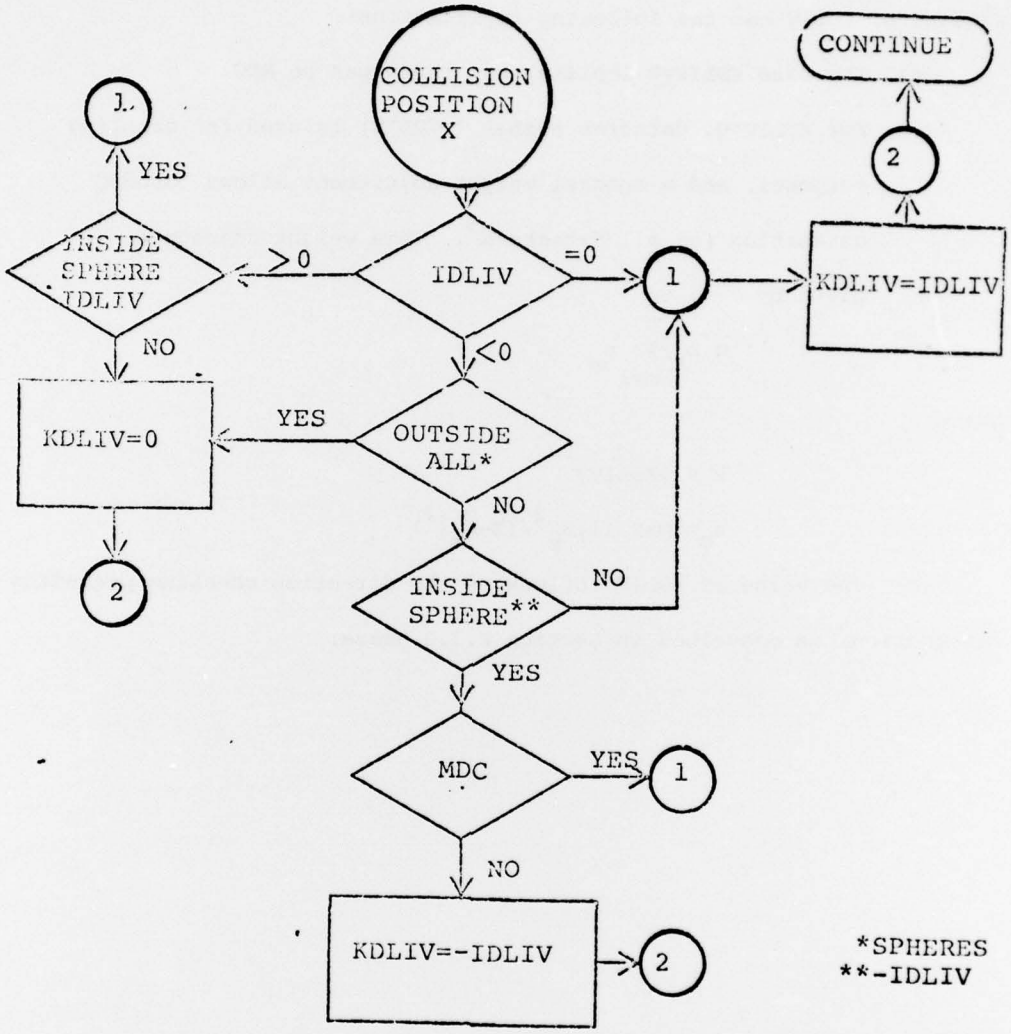

FIGURE F-3

Collision Position Checking Algorithms

F.3.4 Interpretation of KDLIV

As a result of position checking, both for a source and a collision, the setting of KDLIV has the following implications:

(a) The case KDLIV$\geq$0 implies that there was no MDC.

(b) For KDLIV<0, detector number (-KDLIV) is used for sampling purposes, and a special weight adjustment allows bounded estimation for all detectors[5]. This weight adjustment is given by

$$n\, b_k / \sum_{m=1}^{n} b_m$$

where

$$k = |\text{KDLIV}|$$

$$b_m = \max\left(1, R_m^2 / |\bar{x} - \bar{x}_m|^2\right)$$

(c) The value of KDLIV influences the direction checking preceding angle reselection, as described in Section F.3.2 above.

APPENDIX G

"LOWER BOUND" FOR BOUNDED ESTIMATOR

G.1 Introduction

Steinberg[3] introduced a collision selection-reselection technique which guarantees that the estimates to a point detector are bounded from above. If optimum importance sampling is used, all estimates to the detector should be of the order of

$$Q = W(D,E)/4\pi R_c^2 \qquad (G\text{-}1)$$

where W(D,E) is the region and energy dependent weight in the detector region, at the energy of the estimate, and R_c is the radius of the "critical sphere" around the detector (distance corresponding to one m.f.p.)*.

As the importance sampling actually used is often quite different from the optimum one, the individual estimates will fluctuate around the mean. In order to speed up the calculation, we introduce a low value cutoff, below which estimates are Russian-rouletted. The low value cutoff has been chosen to be QxF_o, where F_o is the same as F_z, an input cutoff value relative to unity, used in other parts of the code.

G.2 Implementation

The quantity to be scored is of the form:

$$S = Ge^{-\lambda} \qquad (G\text{-}2)$$

where G reflects all biasing and the $1/r^2$ factor, and is the optical distance from a point to the detector. We rewrite (G-2) as

$$S = Qe^{-(\lambda+\lambda_o)} \qquad (G\text{-}3)$$

where Q is given by Eq. (G-1) and

$$\lambda_o = -\log\ (G/Q) \qquad (G\text{-}4)$$

---

* To safeguard against poor importance sampling, $R_c = \max\ (R_c, r)$, where r is the distance between particle position and detector.

We further define a m.f.p. cutoff value

$$\lambda_c = -\log (F_o) \qquad \text{(G-5)}$$

and replace the test $S < QxF_o$ (G-6)

by the test $\lambda + \lambda_o > \lambda_c$ (G-7)

The optical distance λ is calculated by tracking as a cumulative sum of non-negative terms.

$$\lambda = \lambda^n, \text{ where}$$
$$\lambda^k = \sum_{i=0}^{k} \lambda_i$$

with $\lambda_i > 0$ for $i > 0$.

The test (G-7) is performed by testing

$$\lambda^k > \lambda_c \qquad \text{(G-8)}$$

for k=0,1...

until either the test is satisfied, or k=n, whichever occurs first. If the test is satisfied, a game of chance is played. With probability $1-F_o$, the estimator becomes 0 and the tracking is terminated. With probability F_o, the estimator is multiplied by $1/F_o$ (which is achieved by replacing λ^k by $\lambda^k-\lambda_c$), the tracking and test (G-8) continues for succeeding values of k.

APPENDIX H

ENERGY RANGE HIERARCHY

The principal energy range for a given SAMCEP run is the Monte Carlo tracking range, as specified in the SAMCAR input by EHIGH and ECUT (see Item 11, Section 5.3). The other major energy ranges are defined, relative to (EHIGH, ECUT), as follows:

MONTE CARLO

a) $EOUT_1 > EHIGH > ECUT > EOUT_{LAST}$

where $(EOUT_1, EOUT_{LAST})$ is the output energy range for scoring (Item 12, Section 5.3);

b) $ES_1 > EHIGH > ECUT > ES_{LAST}$

where (ES_1, ES_{LAST}) is the source energy range (Item 25, Section 5.3);

c) $EWTAB_1 > EHIGH > ECUT > EWTAB_{LAST}$

where $(EWTAB_1, EWTAB_{LAST})$ is the energy importance range (Item 17, Section 5.3);

NOTE: There is no hierarchy established among EOUT, ES, and EWTAB.

DATA

d) EEHIGH > EHIGH > ECUT > EELOW

where (EEHIGH,EELOW) is the maximum energy range defined by perturbation input (Item 1, Section 3.2);

e) $EX_1 > EEHIGH > EELOW > EX_{LAST}$

where (EX_1, EX_{LAST}) is the minimum cross section energy range (SAM-X output) utilized in the problem (including type 2 perturbations).

APPENDIX I

OPERATING INSTRUCTIONS FOR SAMCEP

SAMCEP is currently operational under the SCOPE 2.1 system on the CDC 7600. A card deck configuration, assuming the five executable programs comprising the SAMCEP system reside on a permanent file SAMCEP, is shown below:

CARD CONTENTS	COMMENTS
SBLMJ,3TMFZ.	7600 JOB card.
ATTACH(SAMIN,SAMCEP,CY=1)	
SAMIN.	Execute the neutron perturbation processor.
REWIND(TAPE8)	Processed perturbation data tape.
ATTACH(TAPE11,NEDT,CY=1)	Neutron element data generated by SAM-X.
ATTACH(SAMSAM,SAMCEP,CY=2)	
SAMSAM.	Execute the neutron transport preprocessor.
REWIND(TAPE8,TAPE10,TAPE12)	TAPE8 is the modified perturbation data tape; TAPE10 is the organized data tape (ODT output of BAND); TAPE12 is the sampling CHI-and/or ENN-table tape (if any).
RETURN(TAPE11)	
ATTACH(SAMCAR,SAMCEP,CY=3)	
SAMCAR .	Execute the correlated Monte Carlo transport code for the primary neutron problem.
RETURN(TAPE10)	The neutron ODT may also be saved for future neutron runs.
RETURN(TAPE12)	The sampling tape may also be saved for future neutron runs.

CARD CONTENTS	COMMENTS
REWIND(TAPE8,TAPE14,TAPE16)	TAPE8 is needed for a secondary gamma problem; TAPE14 may contain non-elastic neutron interactions from which a secondary gamma source is generated; TAPE16 is the statistical aggregate tape for the primary neutron problem.
ATTACH(SAMOUT,SAMCEP,CY=4)	
SAMOUT(TAPE16)	Execute the edit code (TAPE16 is denoted TAPE1 internally).
RETURN(TAPE16)	
RETURN(TAPE4)	TAPE4, the statistical tape generated by SAMOUT, may be saved for future reruns of SAMOUT.
ATTACH(TAPE11,GEDT,CY=1)	Gamma element data tape generated by SAM-X.
ATTACH(TAPE12,GPDT,CY=1)	Gamma production data tape generated by SAM-X.
ATTACH(SAMGAM,SAMCEP,CY=5)	
SAMGAM.	Execute the secondary gamma preprocessor.
REWIND(TAPE8,TAPE10,TAPE15)	TAPE8 has been modified by SAMGAM, retaining only concentration perturbations from the primary neutron problem; TAPE10 is now the organized gamma cross section data; TAPE15 is the external secondary gamma source tape generated by SAMGAM from the TAPE14, TAPE12, and user supplied data.
RETURN(TAPE12,TAPE14)	

CARD CONTENTS	COMMENTS
SAMCAR.	Execute the correlated Monte Carlo transport code for the secondary gamma problem.
REWIND(TAPE16)	*TAPE16 now contains* statistical aggregates for the secondary gamma problem.
SAMOUT(TAPE16)	Edit the secondary gamma results.
(eor)	
data deck for SAMIN	
(eor)	
data deck for SAMSAM	
(eor)	
data deck for primary neutron SAMCAR	
(eor)	
data deck for primary neutron SAMOUT	
(eor)	
data deck for SAMGAM	
(eor)	
data deck for secondary gamma SAMCAR	
(eor)	
data deck for secondary gamma SAMOUT	
(eof)	

- End of Job Deck -

These programs can be run in separate jobs by saving the appropriate tape files. The following table specifies the required files for each program execution:

TO START WITH	FILES REQUIRED
SAMIN	None
SAMSAM	TAPE8 from SAMIN; TAPE11 (NEDT) from SAM-X.
SAMCAR	TAPE8, TAPE10, TAPE12 from SAMSAM (for primary neutron); TAPE8, TAPE10, TAPE15 from SAMGAM (for secondary gamma) .
SAMOUT	TAPE16 from SAMCAR or TAPE4 from previous SAMOUT.
SAMGAM	TAPE8 from SAMSAM; TAPE14 from primary neutron SAMCAR; TAPE11 (GEDT), TAPE12 (GPDT) from SAM-X.

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